14782048 PASCAL No.: 00-0461702

O-methylation of tea polyphenols catalyzed by human placental cytosolic catechol-O-methyltransferase

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Journal: Drug metabolism and disposition, 2000, 28 (9) 1024-1030

Language: English

In the present study, we evaluated the metabolic O-methylation of several catechol-containing tea polyphenols by human placental catechol-O-methyltransferase (COMT). (-)-Epicatechin, (+)-epicatechin, and (-)-epigallocatechin were good substrates for metabolic O-methylation by placental cytosolic COMT (150-500 pmol/mg of protein/min), but (-)-epicatechin gallate and (-)-**epigallocatechin gallate** were O-methylated at much lower rates (<50 pmol/mg of protein/min). When (-)-epicatechin was used as substrate, its O-methylation by human placental COMT showed dependence on incubation time, cytosolic protein concentration, incubation pH, and concentration of S-adenosyl-L-methionine (the methyl donor). Analysis of cytosolic COMT from six human term placentas showed that the O-methylation of increasing concentrations of (-)-epicatechin or (-)-epigallocatechin follows typical Michaelis-Menten kinetics, with K SUB m and V SUB m SUB a SUB x values of 2.2 to 8.2 mu M and 132 to 495 pmol/mg of protein/min for (-)-epicatechin and 3.9 to 6.7 mu M and 152 to 310 pmol/mg of protein/min for (-)-epigallocatechin, respectively. Additional analysis revealed that COMT-catalyzed O-methylation of (-)-epicatechin and (-)-epigallocatechin was strongly inhibited in a concentration-dependent manner by S-adenosyl-L-homocysteine (IC SUB 5 SUB 0 = 3.2-5.7 mu M), a demethylated product of S-adenosyl-L-methionine. This inhibition by S-adenosyl-L-homocysteine follows a mixed (competitive plus noncompetitive) mechanism of enzyme inhibition. In summary, several **catechol** -containing tea polyphenols are rapidly O-methylated by human placental cytosolic COMT. This metabolic O-methylation is subject to strong inhibitory regulation by S-adenosyl-L-homocysteine, which is formed in large quantities during the I O-methylation of tea polyphenols.

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51 muM and 2882 pmol mg proteinSUP-1 minSUP-1, respectively, at pH7.4, and were 17 muM and 2093 pmol mg proteinSUP-1 minSUP-1, respectively, at pH 10.0. 3. Under optimized conditions for in vitro O-methylation, (-)-epicatechin, (+)-epicatechin and (-)-epigallocatechin were rapidly O-methylated by rat liver cytosol. In comparison, (-)-epicatechin gallate and (-)-**epigallocatechin gallate** were O-methylated at significantly lower rates under the same reaction conditions. 4. COMT-catalysed O-methylation of (-)-epicatechin and (-)-epigallocatechin was inhibited in a concentration-dependent manner by S-adenosyl-L-homocysteine, a demethylated product of S-adenosyl-L-methionine. The ICSUB50 was (similar) 10 muM. 5. In summary, the results showed that several **catechol**-containing tea polyphenols were rapidly O-methylated by rat liver cytosolic COMT. These observations raise the possibility that some of the biological effects of tea polyphenols may be exerted by their O-methylated products or may result from their potential inhibition of the COMT-catalysed O-methylation of endogenous **catecholamines** and **catechol** oestrogens.

9/AB/32 (Item 1 from file: 144)
DIALOG(R)File 144:Pascal

16266664 PASCAL No.: 03-0429187
Enzymology of methylation of tea catechins and inhibition of catechol-O-methyltransferase by (-)-**epigallocatechin gallate**
HONG LU; XIAOFENG MENG; YANG Chung S
Department of Chemical Biology, Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey, Piscataway, New Jersey, United States
Journal: Drug metabolism and disposition, 2003, 31 (5) 572-579
Language: English
(-)-Epigallocatechin gallate (EGCG) and (-)-epigallocatechin (EGC) are the major polyphenolic constituents in green tea. In this study, we characterized the enzymology of cytosolic **catechol** -O-methyltransferase (COMT)-catalyzed methylation of EGCG and EGC in humans, mice, and rats. At 1 mu M, EGCG was readily methylated by liver cytosolic COMT to 4"-O-methyl-EGCG and then to 4',4"-di.O.methyl-EGCG; EGC was methylated to 4'-O-methyl-EGC. The K SUB m and V SUB m SUB a SUB x values for EGC methylation were higher than EGCG; for example, with human liver cytosol, the K SUB m were 4.0 versus 0.16 mu M and V SUB m SUB a SUB x were 1.28 versus 0.16 nmol/mg/min. Rat liver cytosol had higher COMT activity than that of humans or mice. The small intestine had lower specific activity than the liver in the methylation of EGCG and EGC. Glucuronidation on the B-ring or the D-ring of EGCG greatly inhibited the methylation on the same ring, but glucuronidation on the A-ring of EGCG or EGC did not affect their methylation. Using EGC and 3,4-dihydroxy-L-phenylalanine as substrates, EGCG, 4"-O-methyl-EGCG, and 4',4"-di-O-methyl-EGCG were all potent inhibitors (lC SUB 5 SUB 0 similar 0.2 mu M) of COMT. The COMT-inhibiting activity of (-)-EGCG-3'-O-glucuronide was similar to EGCG, but (-)-EGCG-4"-O-glucuronid e was less potent. The present work provides basic information on the methylation of EGCG and suggests that EGCG may inhibit COMT-catalyzed methylation of endogenous and exogenous compounds.

9/AB/33 (Item 2 from file: 144)
DIALOG(R)File 144:Pascal

inhibit carcinogenesis. However, the mechanisms by which green tea extract exerts its anticarcinogenic effect are not yet clearly understood. We have examined the effect of tea polyphenols on polyamine metabolism and the mechanism of its antitumor activity in Ehrlich ascites tumor cells, Ornithine decarboxylase (ODC) activity was measured by estimating the release-of (CO2)-C-14 from L[1-C-14] ornithine,

The amount of ODC mRNA was measured by Northern-blot analysis,

The polyphenols decreased DNA synthesis and cell viability in a dose-dependent manner, The increase in ODC activity caused by changing the medium was inhibited by adding tea polyphenols, The inhibition of the enzyme was dependent on the structure of tea polyphenols. (-)-epigallocatechin and (-)- **epigallocatechin gallate** were effective,, but(+)-catechin, (-)-epicatechin and (-)-epicatechin gallate did not inhibit ODC; induction, suggesting that pyrogallol-type catechins inhibit the enzymic activity of ODC whereas **catechol** -type catechins are less inhibitory, ODC was : not inhibited by tea polyphenols when they were added to the Culture medium 2h after a change to fresh medium. Incubating the cells for 4h with tea polyphenols then washing them out did not recover ODC activity. The ODC mRNA level in the cells treated with green tea extract was comparable to that in the control cells,

These results confirm that green tea extract inhibits ODC induction dose-dependently in Ehrlich ascites tumor cells and that the inhibition of its induction was dependent on the structure of the tea polyphenols, We found that the tea polyphenols caused a marked decrease in ODC activity with no detectable effect on ODC mRNA levels in the cells, suggesting that tea polyphenols inhibit ODC induction at the post-transcriptional level.

9/AB/31 (Item 1 from file: 71)
DIALOG(R)File 71:ELSEVIER BIOBASE

01940471 2002020800
Rapid conversion of tea catechins to monomethylated products by rat liver cytosolic catechol-O-methyltransferase
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EMAIL: BTZhu@cop.sc.edu
Journal: Xenobiotica, 31/12 (879-890), 2001, United Kingdom
CODEN: XENOB
ISSN: 0049-8254
DOCUMENT TYPE: Article
LANGUAGES: English SUMMARY LANGUAGES: English
NO. OF REFERENCES: 27

1. The metabolic O-methylation of several **catechol**-containing tea polyphenols by rat liver cytosolic **catechol**-O-methyltransferase (COMT) has been studied. 2. When (-)-epicatechin was used as substrate, its O-methylation showed dependence on incubation time, cytosolic protein concentration, incubation pH and concentration of S-adenosyl-L-methionine. The O-methylation of increasing concentrations of (-)-epicatechin followed typical Michaelis-Menten kinetics, and the apparent KSUBm and VSUBmax were

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Journal: JOURNAL OF THE CHEMICAL SOCIETY-PERKIN TRANSACTIONS 2, 1998, N11 (NOV), P2365-2369
ISSN: 0300-9580 Publication date: 19981100
Publisher: ROYAL SOC CHEMISTRY, THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON ROAD, CAMBRIDGE CB4 4WF, CAMBS, ENGLAND
Language: English Document Type: ARTICLE
Abstract: Iron(III) complexes of gallocatechins were studied in aqueous Solutions by UV-VIS spectrometry, HPLC, cyclic voltammetry, laser photolysis and pulse radiolysis techniques. The blue-violet colored complexes are readily formed in water. The Job plots indicate 1:1 stoichiometry for the reaction of iron(III) with gallocatechins and methyl gallate, and 1:3 for that of iron(III) and catechin. This suggests that the three phenol groups of the gallate moiety play a role in complex formation. The formation constants of the complexes are found to be pH dependent, as expected for polyhydroxybenzene derivatives. pK(a1) = 4.3 and pK(a2) = 7.4 for the polyphenols with the gallate ester moiety (**epigallocatechin gallate** and epicatechin gallate) are lower than those of epigallocatechin (EGC) and catechin (pK(a1) = 4.9 and pK(a2) = 8.4), very probably because of the electron-withdrawing effect of the ester. Apparent stability constants of iron(III) gallocatechin complexes are high at pH 7, log K approximate to 27, comparable to those of the **catechol** derivatives. Photoionization of the iron complexes by the 248 nm laser is more efficient at higher pH, phi = 0.13 at pH 7 vs. phi = 0.26 at pH 11.5. The absorption spectra, which resemble those of ligand phenoxyl radicals, indicate that photoionization yields unstable phenoxyls, t(1/2) similar to 1 ms. Similar spectra are recorded when one-electron oxidation by the azide radical, N-3(.), is used to generate the ligand radicals. The reduction potential of Fe(III)gallocatechins is -0.325 V vs. NHE, which is similar to 0.45 V less negative than the reduction potential of the Fe(II)/Fe(III) couple. In the case of the catechins with the gallate ester moiety,namely EGCG and ECG,the high pH cyclic voltammograms exhibit a quasi-reversible oxidation-reduction not seen in the other derivatives. The relevance of these findings for the physiological function and antioxidant and chemopreventive action of gallocatechins Is discussed.

9/AB/30 (Item 4 from file: 34)
DIALOG(R)File 34:SciSearch(R) Cited Ref Sci

04957007 Genuine Article#: UV180 Number of References: 37
Title: PREVENTION OF ORNITHINE DECARBOXYLASE INDUCTION IN EHRLICH ASCITES, TUMOR-CELLS BY TEA POLYPHENOLS (Abstract Available)
Author(s): WADATANI M; OHTANI K; KAGEYAMA K; YANO Y; HASUMA T; OTANI S; SAKANAKA S; KIM H; MATSUIYUASA I
Corporate Source: FAC HUMAN LIFE SCI,DEPT FOOD & NUTR,SUMIYOSHI KU,3-3-138 SUGIMOTO/OSAKA 558//JAPAN/; FAC HUMAN LIFE SCI,DEPT FOOD & NUTR,SUMIYOSHI KU/OSAKA 558//JAPAN/; OSAKA UNIV,SUMIYOSHI KU/OSAKA//JAPAN/; OSAKA CITY UNIV,SCH MED,RADIOISOTOPE CTR,ABENO KU/OSAKA 545//JAPAN/; OSAKA CITY UNIV,SCH MED,DEPT BIOCHEM,ABENO KU/OSAKA 545//JAPAN/; TAIYO KAGAKU CO LTD,CENT RES LABS/YOKKAICHI//JAPAN/
Journal: CANCER JOURNAL, 1996, V9, N3 (MAY-JUN), P161-167
ISSN: 0765-7846
Language: ENGLISH Document Type: ARTICLE
Abstract: Green tea extract and some components of green tea are known to

postmenopausal Chinese women in Singapore. In this group of 130 women, 84 were non or irregular (less than once a week) tea drinkers, 27 were regular (weekly/daily) green tea drinkers and 19 were regular (weekly/daily) black tea drinkers. Relative to plasma estrone levels in non- or irregular tea drinkers (29.5 pg/ml) the levels were 13% lower in regular green tea drinkers (25.8 pg/ml) and 19% higher in regular black tea drinkers (35.0 pg/ml). These differences in estrone levels were statistically significant (P = 0.03) inspite of adjusting for age, body mass index, intake of soy, and other covariates. A similar pattern of differences between tea intake, and plasma levels of estradiol (P = 0.08) and androstenedione (P = 0.14) were found. In addition, the tea-estrogen associations were observed irrespective of the genotype of catechol-O-methyltransferase (COMT), a major enzyme that aids in the excretion of tea polyphenols in humans. Larger studies are needed to confirm results from this cross-sectional study and to better understand the potentially differing effect of black and green tea on circulating estrogen levels and ultimately on the risk of breast cancer.

9/AB/28 (Item 2 from file: 34)
DIALOG(R)File 34:SciSearch(R) Cited Ref Sci

13713935 Genuine Article#: 903NZ Number of References: 68
Title: Green tea polyphenols and cancer chemoprevention: Multiple mechanisms and endpoints for phase II trials (ABSTRACT AVAILABLE)
Author(s): Moyers SB (REPRINT) ; Kumar NB
Corporate Source: H Lee Moffitt Canc Ctr & Res Inst,Dept Canc Control & Nutr,Tampa//FL/33606 (REPRINT); H Lee Moffitt Canc Ctr & Res Inst,Dept Canc Control & Nutr,Tampa//FL/33606; Univ Tampa,Tampa//FL/33606; Univ S Florida,Coll Med,Tampa//FL/33606
Journal: NUTRITION REVIEWS, 2004, V62, N5 (MAY), P204-211
ISSN: 0029-6643 Publication date: 20040500
Publisher: INT LIFE SCIENCES INST NORTH AMERICA, ONE THOMAS CIRCLE, N W, 9TH FLOOR, WASHINGTON, DC 20005 USA
Language: English Document Type: REVIEW
Abstract: Among the numerous polyphenols isolated from green tea, the catechin EGCG predominates and is the target of anticancer research. But studies suggest that EGCG and other catechins are poorly absorbed and undergo substantial biotransformation to species that include glucuronides, sulfates, and methylated compounds. Numerous studies relate the antioxidant properties of the catechins with anticancer effects, but recent research proposes other mechanisms of action, including those involving methyl transfers that are subject to allelic variability in the enzyme catechol O-methyl transferase. However, preclinical research is promising and EGCG appears to be ready for further study in phase II and III trials.

9/AB/29 (Item 3 from file: 34)
DIALOG(R)File 34:SciSearch(R) Cited Ref Sci

07239473 Genuine Article#: 140LU Number of References: 41
Title: Iron complexes of gallocatechins. Antioxidant action or iron regulation? (ABSTRACT AVAILABLE)
Author(s): Jovanovic SV (REPRINT) ; Simic MG; Steenken S; Hara Y
Corporate Source: INT CTR METAB TESTING,1305 RICHMOND RD/OTTAWA/ON K2B 7Y4/CANADA/ (REPRINT); TECHLOGIC,/GAITHERSBURG//MD/20877; MAX PLANCK

LANGUAGE: English

ABSTRACT: To screen carcinostatic components in foodstuffs, the toxicity of tea polyphenols was compared between rat 3Y1 diploid fibroblasts and a variety of their vitally transformed cells. Among tea polyphenols tested, epigallocatechin gallate killed 3Y1 cells transformed by E1A gene of human adenovirus type 12 (E1A-3Y1 cells) at a 100 times lower concentration than the parental 3Y1 cells. Epigallocatechin gallate also exerted a strong E1A-3Y1 cell-specific toxicity, while epicatechin and epicatechin gallate did not. When the activity of three antioxidant enzymes was compared between 3Y1 and its transformants, catalase activity was markedly low in the latter, especially in E1A-3Y1 cells, and the substrate of the enzyme, hydrogen peroxide, exerted a toxicity specific to this cell line. Then the inhibitory activities of various chemicals on E1A-3Y1 cell-specific toxicity of phospholipids or **catechol** were examined. Among lipoxygenase inhibitors, all of the polyphenolic compounds inhibited the toxicity of phospholipids, but not a nonpolyphenolic inhibitor (clofibrate). Two phospholipase A-2 inhibitors (dexamethasone and quinacrine) did not inhibit the toxicity. These results indicate that the triphenol structure of the B ring is essential for the E1A-3Y1 cell-specific toxicity of tea polyphenols, and that the decrease in catalase activity is partially responsible for the higher sensitivity of E1A-3Y1 cells against the polyphenols. The inhibitory effect of polyphenolic lipoxygenase inhibitors is ascribed at least in part to their antioxidant activities.

9/AB/27 (Item 1 from file: 34)
DIALOG(R)File 34:SciSearch(R) Cited Ref Sci

13889125 Genuine Article#: 921RE Number of References: 21
Title: Tea and circulating estrogen levels in postmenopausal Chinese women in Singapore (ABSTRACT AVAILABLE)
Author(s): Wu AH (REPRINT) ; Arakawa K; Stanczyk FZ; Van Den Berg D; Koh WP ; Yu MC
Corporate Source: Univ So Calif,Kenneth Norris Jr Comprehens Canc Ctr, Keck Sch Med, Dept Prevent Med,1441 Eastlake Ave/Los Angeles//CA/90089 (REPRINT); Univ So Calif,Kenneth Norris Jr Comprehens Canc Ctr, Keck Sch Med, Dept Prevent Med,Los Angeles//CA/90089; Univ So Calif,Keck Sch Med, Dept Obstet & Gynecol,Los Angeles//CA/90089; Univ So Calif,Keck Sch Med, Dept Urol,Los Angeles//CA/90089; Natl Univ Singapore,Fac Med, Dept Community Occupat & Family Med,Singapore 117597//Singapore/(annawu@usc.edu)
Journal: CARCINOGENESIS, 2005, V26, N5 (MAY), P976-980
ISSN: 0143-3334 Publication date: 20050500
Publisher: OXFORD UNIV PRESS, GREAT CLARENDON ST, OXFORD OX2 6DP, ENGLAND
Language: English Document Type: ARTICLE
Abstract: The role of tea in the etiology of breast cancer is controversial. We recently provided the first set of human evidence that breast cancer risk is significantly inversely associated with tea intake, largely confined to intake of green tea. Since black tea and green tea possess comparable levels of the total tea polyphenols that possess antioxidative activities, reasons for the paradoxical effects of green tea and black tea on breast cancer protection are not apparent. Some limited evidence suggests that green tea may have downregulatory effects on circulating sex-steroid hormones, whereas black tea may have upregulatory effects. We therefore, investigated the relationship between tea intake, and plasma estrogen and androstenedione levels in a cross-sectional study of healthy

were established as catechol, gallic and gentisic acids, gallocatechin (GC) and **epigallocatechin gallate** (EGCG). The main component of polyphenols was **catechol**. On the other hand, very small quantities of the GC and EGCG existed in barley tea. Barley tea and ethyl acetate extract obtained from barley tea showed preventive effects on oxidative deterioration of oil. Especially, ethyl acetate extract were markedly higher than that barley tea. Antioxidant activity of gentisic and gallic acids showed a greater preventive effect.

9/AB/25 (Item 10 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0011684297 BIOSIS NO.: 199800478544
Radical scavenging activity and antimutagenicity of proanthocyanidins from barley bran
AUTHOR: Tamagawa Koji (Reprint); Iizuka Takashi (Reprint); Kobori Masuko; Shinmoto Hiroshi; Tsushida Tojiro
AUTHOR ADDRESS: Res. Dev. Cent., Hakubaku Co. Ltd., 3492 Aoyagi, Masuho-cho, Yamanashi 400-0502, Japan**Japan
JOURNAL: Nippon Shokuhin Kagaku Kogaku Kaishi 45 (7): p420-425 1998 1998
MEDIUM: print
ISSN: 1341-027X
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: Japanese

ABSTRACT: The purpose of this investigation was to clarify the properties of antioxidative activity and antimutagenicity in vitro of proanthocyanidins (dimer and trimer) from barley bran in comparison with catechins. Radical scavenging activities to superoxide and DPPH radical of the prodelphinidins were found to be higher than those of the procyanidins, and almost the same as those of (-) -epigallocatechin ((-)-EGC) and (-)-epigallocatechin gallate ((-)-EGCG). The prodelphinidins from barley bran showed more effective antimutagenicity to MNNG and Trp-p-1 than that of the procyanidins, and showed the same or less effectiveness than those of (-)-EGCG and (-)-EGC. These results suggested that the B-rings with three hydroxyl groups (pyrogallol-type) such as prodelphinidins, (-)-EGC, and (-)-EGCG were more effective to antioxidative activity and antimutagenicity than the B-rings with two hydroxyl groups (**catechol**-type) such as procyanidins, catechin, (-)-epicatechin, and (-)-epicatechin gallate.

9/AB/26 (Item 11 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0009675064 BIOSIS NO.: 199598142897
E1A-3Y1 cell specific toxicity of tea polyphenols and their killing mechanism
AUTHOR: Mitsui Takeshi; Yamada Koji (Reprint); Yamashita Kouhei; Matsuo Noritaka; Okuda Atsuyuki; Kimura Genki; Sugano Michihiro
AUTHOR ADDRESS: Lab. Food Sci. Technol., Fac. Agric., Kyushu Univ. 46-09, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812, Japan**Japan
JOURNAL: International Journal of Oncology 6 (2): p377-383 1995 1995
ISSN: 1019-6439
DOCUMENT TYPE: Article
RECORD TYPE: Abstract

AUTHOR ADDRESS: Department of Food Chemistry, University College, Cork, Ireland**Ireland
JOURNAL: Journal of Dairy Research 66 (3): p399-407 Aug., 1999 1999
MEDIUM: print
ISSN: 0022-0299
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: A methanol extract of green tea was fractionated on Sephadex LH-20. The compounds eluted were identified by thin layer chromatography as catechin-epicatechin, gallocatechin, epigallocatechin, epicatechin gallate and epigallocatechin gallate. When added to milk at 2.0 g/l, these polyphenols, apart from the catechin-epicatechin mixture, increased the heat stability of skim milk, particularly in the region of the minimum (pH 6.8-7.1). When added at 0.4 g/l, green tea polyphenols also increased the heat stability of concentrated milk. The effects of other phenolic compounds on the heat stability of milk were also examined. Chlorogenic acid, guaiacol, thymol, vanillin, butylene hydroxyanisole, propyl gallate and butylene hydroxytoluene did not affect the heat stability of milk or concentrated milk. Quinic acid markedly reduced the heat stability of skim milk. Pyrogallol, **catechol**, tannic acid, ellagic acid, phloroglucinol and gallate converted a type A heat coagulation time-pH profile to atype B profile. Ferulic acid and vanillic acid increased heat stability in the region of the maximum, with little effect on the minimum, and stability did not recover at pH values on the alkaline side of the minimum. Caffeic acid increased the heat stability of milk while the related non-phenolic compounds 2,5-dimethoxycinnamic acid and 3,4-dimethoxycinnamic acid had no effect.

9/AB/24 (Item 9 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0011966803 BIOSIS NO.: 199900226463
Antioxidant activity of barley tea and their composition
AUTHOR: Kajimoto Goro (Reprint); Onitake Naoko (Reprint); Okuda Hiroko (Reprint); Murakami Chikako (Reprint)
AUTHOR ADDRESS: Faculty of Nutrition, Kobe Gakuin University, Arise, Ikawadai-cho, Nishi-ku, Kobe-shi, 651-2113, Japan**Japan
JOURNAL: Nippon Shokuhin Kagaku Kogaku Kaishi 46 (2): p67-74 1999 1999
MEDIUM: print
ISSN: 1341-027X
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: Japanese

ABSTRACT: In our previous paper, we assessed the antioxidant effect of warm water extract from barley grain on the oxidative deterioration of oil. In the present, antioxidant compositions in hot water extract from barley grain (referred to as barley tea hereafter) were identified, and their antioxidant activity was measured. Polyphenols in barley tea were identified by using high performance liquid chromatography (column, Develosil ODS-HG, mobile phase, distilled water-acetonitrile-0.05 M phosphoric acid 90 : 10 : 0.05 v/v), thin-layer chromatography (the fraction by silicagel G 60) and ultra violet spectrum analysis. Antioxidant activity was assessed by the Rancimat method so as to determine the rancid point (induction time) and the oven test. Polyphenols in barley tea was detected, and the structures of polyphenols

macroloba approximately double amounts from H. opuntia. Other polyphenolic compounds tested in this study were not found from both Halimeda.

9/AB/22 (Item 7 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0013111903 BIOSIS NO.: 200100283742
Structure-activity relationship of antioxidants for inhibitors of linoleic acid hydroperoxide-induced toxicity in cultured human umbilical vein endothelial cells
AUTHOR: Kaneko Takao (Reprint); Baba Naomichi; Matsuo Mitsuyoshi
AUTHOR ADDRESS: Tokyo Metropolitan Institute of Gerontology, 35-2 Sakaecho, Itabashi-ku, Tokyo, 173-0015, Japan**Japan
JOURNAL: Cytotechnology 35 (1): p43-55 January, 2001 2001
MEDIUM: print
ISSN: 0920-9069
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: Structure-activity relationship of antioxidants for the protective effects on linoleic acid hydroperoxide (LOOH)-induced toxicity were examined in cultured human umbilical vein endothelial cells. alpha-Tocopherol, 2,2,5,7,8-pentamethylchroman-6-ol, butylated hydroxytoluene, probucol, and fatty acid esters of ascorbic acid provided efficient protection against the cytotoxicity of LOOH in pretreatment, but phenols without alkyl groups at the ortho positions and hydrophilic antioxidants such as Trolox and ascorbic acid provided no protection. Probably, the effectiveness of the protection against cytotoxicity by these antioxidants depends primarily on their rate of incorporation into cells due to their lipophilicity, secondly on their antioxidant activity, and thirdly on their orientation in biomembranes. On the other hand, flavones, such as baicalein and luteolin bearing 3 to 5 hydroxyl groups, and flavonols showed a protective effect against LOOH cytotoxicity when added together with LOOH, but not by pretreatment. Among catechins, (+)-catechin and (-)-epigallocatechin gallate monoglucoside and diglucoside were effective in suppressing LOOH-induced cytotoxicity, but their effects were not so strong. The structure-activity relationship of flavonoids revealed the presence of either the ortho-dihydroxy structure in the B ring of flavonoids or the 3-hydroxyl and 4-oxo groups in the C ring to be important for the protective activities. Furthermore, coumarins such as esculetin containing the ortho **catechol** structure had protective effects in both pretreatment and concurrent treatment. These results suggest that ortho **catechol** moiety of flavonoids, catechins, and coumarins is an important structure in the protection against LOOH-induced cytotoxicity, and that the alkyl groups of monophenols are critical for protection.

9/AB/23 (Item 8 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0012174931 BIOSIS NO.: 199900434591
Effects of phenolic compounds on the heat stability of milk and concentrated milk
AUTHOR: O'Connell John E; Fox Patrick F (Reprint)

(Reprint); Hara Yukihiko; Tokuda Harukuni; Nishino Hoyoku; Uesato Shinichi (Reprint)
AUTHOR ADDRESS: Department of Biotechnology, Faculty of Engineering, Kansai University, Suita, Osaka, 564-8680, Japan**Japan
JOURNAL: Natural Medicines 57 (1): p31-33 February 2003 2003
MEDIUM: print
ISSN: 1340-3443
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: Four catechins were assessed for antiproliferative activities against human breast carcinoma cells SKBR3 overexpressing Her2/neu as well as against human colon carcinoma cells SW620, not overexpressing Her2/neu, which serves as a reference. As a result, (-)-epigallocatechin gallate and (-)-epigallocatechin inhibited the growth of SKBR3 cells at nearly the same concentration (IC50 37.7+-5.7muM and 41.7+-9.2 muM, respectively). In contrast, the **catechol**-type catechins: (-)-epicatechin and (+)-catechin showed much lower activities (both IC50>150 muM). Furthermore, no catechins inhibited SW620 cell growth even with 150 muM. These results suggested that not only (-)-**epigallocatechin gallate** but also (-)-epigallocatechin can be a potential candidate for prognostic treatments of breast cancer overexpressing Her2/neu protein.

9/AB/21 (Item 6 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0014148772 BIOSIS NO.: 200300107491
Compositional difference of phenolic compounds between two seaweeds, Halimeda spp.
AUTHOR: Yoshie Yumiko (Reprint); Wang Wei (Reprint); Hsieh Ya-Pei (Reprint); Suzuki Takeshi (Reprint)
AUTHOR ADDRESS: Department of Food Science and Technology, Tokyo University of Fisheries, 5-7, Konan 4-chome, Minato-ku, Tokyo, 108-8477, Japan** Japan
JOURNAL: Journal of the Tokyo University of Fisheries 88 p21-24 March 2002 2002
MEDIUM: print
ISSN: 0040-9014
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: Halimeda macroloba and Halimeda opuntia were collected at their growing district (Ishigaki island, Okinawa Pref., Japan), in the same season. Polyphenolic and related phenolic compounds were extracted from two Halimeda, and analyzed by high performance liquid chromatography. Polyphenolic compounds (catechin, epicatechin, epigallocatechin, catechin gallate, epicatechin gallate, epigallocatechin gallate, rutin, quercitrin, hesperidin, myricetin, morin, luteolin, quercetin, apigenin, kaempferol, baicalein) and related phenolic compounds (caffeic acid and **catechol**) were determined. The composition of polyphenolic and related phenolic compounds was different between two Halimeda. The extremely large amount (28,000mug/g dry matter) of epigallocatechin was found in H. macroloba. Caffeic acid and hesperidin were found only in H. macroloba. **Catechol** was detected in H. macroloba 5 times as much as **catechol** in H. opuntia. Myricetin and morin were found in H.

(skim or full-fat alike) lowered the response more in the teas than in the coffee.

9/AB/19 (Item 4 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0014353771 BIOSIS NO.: 200300311260
Multiple forms of phenol oxidase from Kolkhida tea leaves (Camelia Sinensis L.) and Mycelia Sterilia IBR 35219/2 and their role in tea production.
AUTHOR: Pruidze G N (Reprint); Mchedlishvili N I; Omiadze N T; Gulua L K; Pruidze N G
AUTHOR ADDRESS: Durmishidze Institute of Biochemistry and Biotechnology, Academy of Sciences of Georgia, 380059, Tbilisi, Georgia**Georgia
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JOURNAL: Food Research International 36 (6): p587-595 2003 2003
MEDIUM: print
ISSN: 0963-9969
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: Molecular weights, (MW) pH optimum and substrate specificity of multiple forms of phenol oxidases from Kolkhida tea leaves (Camelia sinensis L.) and microscopic fungus Mycelia sterilia IBR 35219/2 have been studied. It has been shown that Kolkhida tea leaves consist of phenol oxidases with MW 28,000, 41,000, 58,000, 118,000 and 250,000. Duration of M. sterilia IBR 35219/2 cultivation affects formation and activities of multiple forms of phenol oxidases (MW 240,000, 93,000, 58,000 and 41,000) in the culture filtrate. Maximum activity of phenol oxidases is revealed at 36-h duration period of cultivation. By this time Phenol oxidase, mainly, with MW 240,000 is produced. Both Kolkhida tea leaves phenol oxidase with MW 250,000 and M. sterilia IBR 35219/2 phenol oxidase with MW 240,000 are catechol oxidases with similar substrate specificities. Multiple forms of phenol oxidase from tea leaf with MW 118,000+-3000 and 58,000+-2000 do not reveal hydroxylase activity but they intensively catalyze oxidation of o-diphenols. High molecular weight forms of phenol oxidase of both Kolkhida tea leaves (MW 250,000, 118 00 and 58,000) and M. sterilia IBR 35219/2 (MW 240,000) catalyze the oxidation of catechins, mainly (-)epigallocatecin and (-) **epigallocatechin gallate**. Theaflavins and thearubugins produced at this time regulate phenol oxidase activity. High concentration of these products completely inhibits activity of phenol oxidase. Phenol oxidases of low molecular weights (MW 28,000 and 41,000) from tea leaves catalyze hydroxylation of monophenols, namely, p-coumaric acid, producing o-diphenols. Phenol oxidase of microscopic fungus M. sterilia IBR 35219/2 with MW 240,000 catalyzes oxidation of green tea extract polyphenols.

9/AB/20 (Item 5 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0014328116 BIOSIS NO.: 200300285791
Antiproliferative activity of some catechins against Her2/neu-overexpressing human breast carcinoma SKBR3.
AUTHOR: Maeda Taishi (Reprint); Nagaoka Yasuo (Reprint); Kobayashi Shinya

LANGUAGE: English

9/AB/17 (Item 2 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0014579585 BIOSIS NO.: 200300548304
Effect of black tea theaflavins and related benzotropolone derivatives on 12-O-Tetradecanoylphorbol-13-acetate-induced mouse ear inflammation and inflammatory mediators.
AUTHOR: Ramji Divya (Reprint); Sang Shengmin (Reprint); Liu Yue; Rosen Robert T; Ghai Geetha; Ho Chi-Tang (Reprint); Yang Chung S; Huang Mou-Tuan
AUTHOR ADDRESS: Department of Food Science, Rutgers University, 65 Dudley Road, New Brunswick, NJ, 08901-8520, USA**USA
AUTHOR E-MAIL ADDRESS: divya4@eden.rutgers.edu
JOURNAL: Abstracts of Papers American Chemical Society 226 (1-2): pAGFD 38 2003 2003
MEDIUM: print
CONFERENCE/MEETING: 226th ACS (American Chemical Society) National Meeting New York, NY, USA September 07-11, 2003; 20030907
SPONSOR: American Chemical Society
ISSN: 0065-7727 _(ISSN print)
DOCUMENT TYPE: Meeting; Meeting Abstract
RECORD TYPE: Citation
LANGUAGE: English

9/AB/18 (Item 3 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0014495753 BIOSIS NO.: 200300454432
Characterisation of polyphenols in green, oolong, and black teas, and in coffee, using cyclic voltammetry.
AUTHOR: Kilmartin Paul A (Reprint); Hsu Chyong F
AUTHOR ADDRESS: Food Science Programme, Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, New Zealand**New Zealand
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JOURNAL: Food Chemistry 82 (4): p501-512 September 2003 2003
MEDIUM: print
ISSN: 0308-8146
DOCUMENT TYPE: Article
RECORD TYPE: Abstract
LANGUAGE: English

ABSTRACT: Phenolic compounds are important for their astringent taste and as antioxidants in health. Green, oolong and black tea and an instant coffee were each diluted 50 times in a pH 7.0 phosphate buffer and, along with phenolic standards, were analysed by cyclic voltammetry at a carbon electrode. Standards with a pyrogallol group (gallocatechins) were strong reducing agents and produced a peak at 90-120 mV, while those with a catechol or gallate group peaked at 180-220 mV. The response of green and oolong teas was dominated by **epigallocatechin gallate**, and levels determined by HPLC were consistent with the electrochemical response. Black tea behaved like a theaflavin extract, and coffee like 5-O-caffeoylquinic acid, both with peaks at around 230 mV. The level of phenolics increased with water temperature from 20 to 100degreeC, while lower levels were obtained for repeat infusions. The addition of milk

generated from Angeli's salt caused DNA strand breakage, which was also inhibited by flavonoids but at only high concentrations. On the basis of these findings, we propose that NO- and/or peroxynitrite could be responsible for DNA strand breakage induced by NO and a flavonoid having an ortho-trihydroxyl group. Our results indicate that flavonoids have antioxidant properties, but some act as pro-oxidants in the presence of NO.

9/AB/15 (Item 15 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

09070555 PMID: 2381042
[Antibacterial and anti-hemolysin activities of tea catechins and their structural relatives]
Toda M; Okubo S; Ikigai H; Shimamura T
Department of Bacteriology and Immunology, Showa University School of Medicine, Tokyo.
Nippon saikingaku zasshi. Japanese journal of bacteriology (JAPAN) Mar 1990, 45 (2) p561-6, ISSN 0021-4930 Journal Code: 2984804R
Publishing Model Print
Document type: Journal Article ; English Abstract
Languages: JAPANESE
Main Citation Owner: NLM
Record type: MEDLINE; Completed
Among catechins tested, (-)epigallocatechin (EGC), (-)epicatechin gallate (ECg), (-) epigallocatechin gallate (EGCg) inhibited the growth of Staphylococcus aureus, Vibrio cholerae O1 classical Inaba 569B and El Tor Inaba V86. S. aureus was more sensitive than V. cholerae O1 to these compounds. EGCg showed also a bactericidal activity against V. cholerae O1 569B. Pyrogallol showed a stronger antibacterial activity against S. aureus and V. cholerae O1 than tannic and gallic acid. Rutin or caffein had no effect on them. ECg and EGCg showed the most potent anti-hemolysin activity against S. aureus alpha-toxin, Vibrio parahaemolyticus thermostable direct hemolysin (Vp-TDH) and cholera hemolysin. Among catechin relatives, only tannic acid had a potent anti-hemolysin activity against alpha-toxin. These results suggest that the **catechol** and pyrogallol groups are responsible for the antibacterial and bactericidal activities, while the conformation of catechins might play an important role in the anti-hemolysin activity.

9/AB/16 (Item 1 from file: 5)
DIALOG(R)File 5:Biosis Previews(R)

0015396733 BIOSIS NO.: 200510091233
Comparison of CUMC6335 and epigallocatechin gallate on the inhibition of **catecholamine** release in the perfused rabbit adrenal medulla
AUTHOR: Lim Dong-Yoon (Reprint)
AUTHOR ADDRESS: Chosun Univ, Coll Med, Dept Pharmacol, Kwangju, South Korea **South Korea
JOURNAL: Journal of Hypertension 22 (Suppl. 1): pS18 FEB 04 2004
CONFERENCE/MEETING: 20th Scientific Meeting of the International-Society-of-Hypertension Sao Paulo, BRAZIL February 15 -19, 2004; 20040215
SPONSOR: Int Soc Hypertens
ISSN: 0263-6352
DOCUMENT TYPE: Meeting; Meeting Abstract
RECORD TYPE: Citation

Document type: Clinical Trial; Journal Article; Randomized Controlled Trial
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

BACKGROUND: Current interest in the role of functional foods in weight control has focused on plant ingredients capable of interfering with the sympathoadrenal system. OBJECTIVE: We investigated whether a green tea extract, by virtue of its high content of caffeine and catechin polyphenols, could increase 24-h energy expenditure (EE) and fat oxidation in humans. DESIGN: Twenty-four-hour EE, the respiratory quotient (RQ), and the urinary excretion of nitrogen and catecholamines were measured in a respiratory chamber in 10 healthy men. On 3 separate occasions, subjects were randomly assigned among 3 treatments: green tea extract (50 mg caffeine and 90 mg **epigallocatechin gallate**), caffeine (50 mg), and placebo, which they ingested at breakfast, lunch, and dinner. RESULTS: Relative to placebo, treatment with the green tea extract resulted in a significant increase in 24-h EE (4%; $P < 0.01$) and a significant decrease in 24-h RQ (from 0.88 to 0.85; $P < 0.001$) without any change in urinary nitrogen. Twenty-four-hour urinary norepinephrine excretion was higher during treatment with the green tea extract than with the placebo (40%, $P < 0.05$). Treatment with caffeine in amounts equivalent to those found in the green tea extract had no effect on EE and RQ nor on urinary nitrogen or **catecholamines**. CONCLUSIONS: Green tea has thermogenic properties and promotes fat oxidation beyond that explained by its caffeine content per se. The green tea extract may play a role in the control of body composition via sympathetic activation of thermogenesis, fat oxidation, or both.

9/AB/14 (Item 14 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

12554557 PMID: 9870559

Antioxidant and pro-oxidant actions of flavonoids: effects on DNA damage induced by nitric oxide, peroxynitrite and nitroxyl anion.

Ohshima H; Yoshie Y; Auriol S; Gilibert I
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Free radical biology & medicine (UNITED STATES) Dec 1998, 25 (9) p1057-65, ISSN 0891-5849 Journal Code: 8709159
Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

Antioxidant and pro-oxidant activities of flavonoids have been reported. We have studied the effects of 18 flavonoids and related phenolic compounds on DNA damage induced by nitric oxide (NO), peroxynitrite, and nitroxyl anion (NO-). Similarly to our previous findings with catecholamines and catechol-estrogens, DNA single-strand breakage was induced synergistically when pBR322 plasmid was incubated in the presence of an NO-releasing compound (diethylamine NONOate) and a flavonoid having an ortho-trihydroxyl group in either the B ring (e.g., **epigallocatechin gallate**) or the A ring (e.g., quercetagetin). Either NO or any of the above flavonoids alone did not induce strand breakage significantly. However, most of the tested flavonoids inhibited the peroxynitrite-mediated formation of 8-nitroguanine in calf-thymus DNA, measured by a new HPLC-electrochemical detection method, as well as the peroxynitrite-induced strand breakage. NO-

inhibitory regulation by S-adenosyl-L-homocysteine, which is formed in large quantities during the O-methylation of tea polyphenols.

9/AB/12 (Item 12 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

12740620 PMID: 10666317
Electron paramagnetic resonance studies of radical species of proanthocyanidins and gallate esters.
Bors W; Michel C; Stettmaier K
Institut fur Strahlenbiologie, GSF Forschungszentrum fur Umwelt und Gesundheit, Neuherberg, D-85764, Germany. bors@gsf.de
Archives of biochemistry and biophysics (UNITED STATES) Feb 15 2000, 374 (2) p347-55, ISSN 0003-9861 Journal Code: 0372430
Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed
The polyphenols present in green tea or red wine comprise both regular flavon(ol)s and proanthocyanidins, i.e., derivatives of flavan-3-ols, whose distinct antioxidative potential is of great importance for explaining the beneficial effects of these nutrient beverages. Using EPR spectroscopy, we investigated radical structures obtained after oxidation of the parent compounds either by horseradish peroxidase/hydrogen peroxide or after autoxidation in moderately alkaline solutions. Both proanthocyanidins (monomers of condensed tannins, e.g., (+)-catechin, (-)-epicatechin, (-)-epicatechin gallate, (-)-epigallocatechin, (-)-epigallocatechin gallate, Pycnogenol) and gallate esters (hydrolyzable tannins, e.g., propylgallate, beta-glucogallin, pentagalloyl glucose and tannic acid) yielded predominantly semiquinone structures derived from the parent **catechol** or pyrogallol moieties. Evidence for a time-dependent oligomerization was obtained for (-)-**epigallocatechin gallate**, supporting our hypothesis that o-quinones formed from the initial semiquinone disproportionation are prone to nucleophilic addition reactions. Such phenolic coupling reactions would retain the numbers of reactive **catechol** /pyrogallol structures and thus the antioxidative potential. We therefore propose that proanthocyanidins are superior antioxidants as compared to flavon(ol)s proper, whose quinones are more likely to redox-cycle and act as prooxidants. Copyright 2000 Academic Press.

9/AB/13 (Item 13 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

12663743 PMID: 10584049
Efficacy of a green tea extract rich in catechin polyphenols and caffeine in increasing 24-h energy expenditure and fat oxidation in humans.
Dulloo A G; Duret C; Rohrer D; Girardier L; Mensi N; Fathi M; Chantre P; Vandermander J
Department of Physiology, Faculty of Medicine, University of Geneva. abdul.dulloo@unifr.ch
American journal of clinical nutrition (UNITED STATES) Dec 1999, 70 (6) p1040-5, ISSN 0002-9165 Journal Code: 0376027
Publishing Model Print; Comment in Am J Clin Nutr. 2000 Nov;72(5) 1232-4; Comment in PMID 11063454

Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

The Effects of pH on antioxidative activities of catechol, pyrogallol, and four catechins, and effects of metal ions (Al3+, Ca2+, Cd2+, Co2+, Cr3+, Cu2+, Fe2+, Fe3+, K+, Mg2+, Mn2+, Na+, and Zn2+) on antioxidative activities of (-)-**epigallocatechin gallate** (EGCG) were studied by an oxygen electrode method. The antioxidative activities of catechins were high and constant at pH 6-12, but decreased in acidic and strong alkaline solutions. Copper(II) ion the most strongly increased the antioxidative activity of EGCG among these metal ions examined, but iron(II) ion largely inhibited the antioxidative activity of EGCG. These effects are discussed considering the formation of metal complexes with catechins and the change in oxidation potentials.

9/AB/11 (Item 11 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

12994200 PMID: 10950844

O-Methylation of tea polyphenols catalyzed by human placental cytosolic catechol-O-methyltransferase.

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Drug metabolism and disposition- the biological fate of chemicals (UNITED STATES) Sep 2000, 28 (9) p1024-30, ISSN 0090-9556 Journal Code: 9421550

Contract/Grant No.: CA 49756; CA; NCI; CA 74787; CA; NCI; ES 05022; ES; NIEHS

Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

In the present study, we evaluated the metabolic O-methylation of several catechol-containing tea polyphenols by human placental catechol-O-methyltransferase (COMT). (-)-Epicatechin, (+)-epicatechin, and (-)-epigallocatechin were good substrates for metabolic O-methylation by placental cytosolic COMT (150-500 pmol/mg of protein/min), but (-)-epicatechin gallate and (-)-**epigallocatechin gallate** were O-methylated at much lower rates (<50 pmol/mg of protein/min). When (-)-epicatechin was used as substrate, its O-methylation by human placental COMT showed dependence on incubation time, cytosolic protein concentration, incubation pH, and concentration of S-adenosyl-L-methionine (the methyl donor). Analysis of cytosolic COMT from six human term placentas showed that the O-methylation of increasing concentrations of (-)-epicatechin or (-)-epigallocatechin follows typical Michaelis-Menten kinetics, with K(m) and V(max) values of 2.2 to 8.2 microM and 132 to 495 pmol/mg of protein/min for (-)-epicatechin and 3.9 to 6.7 microM and 152 to 310 pmol/mg of protein/min for (-)-epigallocatechin, respectively. Additional analysis revealed that COMT-catalyzed O-methylation of (-)-epicatechin and (-)-epigallocatechin was strongly inhibited in a concentration-dependent manner by S-adenosyl-L-homocysteine (IC(50) = 3.2-5.7 microM), a demethylated product of S-adenosyl-L-methionine. This inhibition by S-adenosyl-L-homocysteine follows a mixed (competitive plus noncompetitive) mechanism of enzyme inhibition. In summary, several **catechol** -containing tea polyphenols are rapidly O-methylated by human placental cytosolic COMT. This metabolic O-methylation is subject to strong

activity and the lower redox potential. The O2-* scavenging activity was well correlated with the Cu2+ reducing ability of flavonoids and aromatics.

9/AB/9 (Item 9 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

14018391 PMID: 11780762
Rapid conversion of tea catechins to monomethylated products by rat liver cytosolic catechol-O-methyltransferase.
Zhu B T; Patel U K; Cai M X; Lee A J; Conney A H
Department of Basic Pharmaceutical Sciences, College of Pharmacy, University of South Carolina, Columbia 29208, USA. BTZhu@cop.sc.edu
Xenobiotica; the fate of foreign compounds in biological systems (England) Dec 2001, 31 (12) p879-90, ISSN 0049-8254 Journal Code: 1306665
Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed
1. The metabolic O-methylation of several catechol-containing tea polyphenols by rat liver cytosolic catechol-O-methyltransferase (COMT) has been studied. 2. When (-)-epicatechin was used as substrate, its O-merthylation showed dependence on incubation time, cytosolic protein concentration, incubation pH and concentration of S-adenosyl-L-methionine. The O-methylation of increasing concentrations of (-)-epicatechin followed typical Michaelis-Menten kinetics, and the apparent Km and Vmax were 51 microM and 2882 pmol mg protein(-1) min(-1), respectively, at pH 7.4, and were 17 microM and 2093 pmol mg protein(-1) min(-1), respectively, at pH 10.0. 3. Under optimized conditions for in vitro O-methylation, (-)-epicatechin, (+)-epicatechin and (-)-epigallocatechin were rapidly O-methylated by rat liver cytosol. In comparison, (-)-epicatechin gallate and (-)-**epigallocatechin gallate** vere O-methylated at significantly lower rates under the same reaction conditions. catalysed O-methylation of (-)-epicatechin and (-)-epigallocatechin was inhibited in a concentration-dependent manner by S-adenosyl-L-homocysteine, a demethylated product of S-adenosyl-L-methionine. The IC50 was approximately 10 microM. 5. In summary, the results showed that several **catechol** -containing tea polyphenols were rapidly O-methylated by rat liver cytosolic COMT. These observations raise the possibility that some of the biological effects of tea polyphenols may be exerted by their O-methylated products or may result from their potential inhibition of the COMT-catalysed O-methylation of endogenous **catecholamines** and **catechol** oestrogens.

9/AB/10 (Item 10 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

13604322 PMID: 11272815
Effects of pH and metal ions on antioxidative activities of catechins.
Kumamoto M; Sonda T; Nagayama K; Tabata M
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Bioscience, biotechnology, and biochemistry (Japan) Jan 2001, 65 (1) p126-32, ISSN 0916-8451 Journal Code: 9205717
Publishing Model Print
Document type: Journal Article

(-)-epigallocatechin gallate (EGCG). EGCG shows potent inhibition in cell-free but not in whole-cell assays of 5 alpha-reductase. Replacement of the gallate ester in EGCG with long-chain fatty acids produced potent 5 alpha-reductase inhibitors that were active in both cell-free and whole-cell assay systems. Other flavonoids that were potent inhibitors of the type 1 5alpha-reductase include myricetin, quercitin, baicalein, and fisetin. Biochanin A, daidzein, genistein, and kaempferol were much better inhibitors of the type 2 than the type 1 isozyme. Several other natural and synthetic polyphenolic compounds were more effective inhibitors of the type 1 than the type 2 isozyme, including alizarin, anthrarobin, gossypol, nordihydroguaiaretic acid, caffeic acid phenethyl ester, and octyl and dodecyl gallates. The presence of a **catechol** group was characteristic of almost all inhibitors that showed selectivity for the type 1 isozyme of 5 alpha-reductase. Since some of these compounds are consumed as part of the normal diet or in supplements, they have the potential to inhibit 5 alpha-reductase activity, which may be useful for the prevention or treatment of androgen-dependent disorders. However, these compounds also may adversely affect male sexual differentiation.

9/AB/8 (Item 8 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

14055490 PMID: 11824550

The contribution of the pyrogallol moiety to the superoxide radical scavenging activity of flavonoids.

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Biological & pharmaceutical bulletin (Japan) Jan 2002, 25 (1) p19-23, ISSN 0918-6158 Journal Code: 9311984

Publishing Model Print

Document type: Journal Article

Languages: ENGLISH

Main Citation Owner: NLM

Record type: MEDLINE; Completed

Sixteen flavonoids including flavonols, flavones, flavanonol and catechins, and five aromatic compounds were examined for their ability to scavenge superoxide radical (O2-*) generated enzymatically in a xanthin-xanthinoxidase system and non-enzymatically in a phenazine methosulfate-NADH system. Pyrogallol, gallic acid and its ester, were much more efficient in scavenging O2-* than catechol. The superiority of pyrogallol over catechol in the flavonoidal nucleus is apparent from the much higher O2-* scavenging activity of myricetin and epigallocatechin, which contain 3',4',5'-trihydroxyl substitution in the B-ring, compared to quercetin and epicatechin, which contain 3',4'-dihydroxyl substitution, respectively. The strong O2-* scavenging ability of pyrogallol appears to function even in the A-ring, as in baicalein, and also in the form of a pyrogalloyl ester at the C-3 position in the C-ring, as in epicatechin gallate and **epigallocatechin gallate**. It can be concluded that the pyrogallol moiety is an active component of flavonoids for displaying high O2-* scavenging activity. Flavonoids and aromatics were also examined to correlate their O2-* scavenging activity with their oxidizability, which was measured on the basis of electrochemical redox potential and the reducing ability of the Cu2+ ion. Aromatics such as pyrogallol, gallic acid and its ester, and flavonoids such as baicalein, epicatechin gallate and **epigallocatechin gallate**, in which the O2-* scavenging activity is enhanced by the presence of a pyrogallol moiety which does not belong to the B-ring, reduced the correlation between the higher O2-* scavenging

Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

Coelenterazine (2-p-hydroxybenzyl-6-(3'-hydroxyphenyl)-8-benzyl-3,7-dihydroimidazolo[1,2-a]pyrazin-3-one, CLZn) and coelenteramine (2-amino-3-benzyl-5-(4'-hydroxyphenyl)-1,4-pyrazine, CLM), first described as luciferin and etioluciferin, respectively, of bioluminescent systems in marine organisms are endowed with antioxidant properties. This study was aimed at understanding the structural basis of their chain-breaking properties and at designing new compounds with improved antioxidative properties. For this, a series of 2-amino-1,4-pyrazine derivatives and their related imidazolopyrazinones were synthesised and examined for their capacity to inhibit lipid peroxidation in linoleate micelles subjected to the peroxidizing action of AAPH. Structure-activity relationship studies indicated that the reduction of the peroxidation rate by CLM is mainly determined by the concomitant presence of 5-p-hydroxyphenyl and 2-amino groups in para position. The lipophilic character of substituents also affected this effect. All imidazolopyrazinones induced a lag-time before the onset of the peroxidation process. The hetero-bicyclic imidazolopyrazinone moiety appears as the main contributor to this activity while phenol groups play little role in it. On the other hand, phenol groups were required for the reduction of the peroxidation rate after the lag-phase. The introduction of a supplementary p-hydroxyphenyl substituent at C8 position did not increase chain-breaking properties. The substitution of the C5-p-hydroxyphenyl with a **catechol** moiety or the introduction of a second amino group on the pyrazine ring yielded the most active compounds, superior to imidazolopyrazinones and reference antioxidants like **epigallocatechin gallate** , vitamin E and trolox. The strong antioxidant properties of 2,6-diaminopyrazines are not dependent on the presence of hydroxyl groups indicating that their reaction mechanism differs from that of 2-amino-1,4-pyrazine derivatives.

9/AB/7 (Item 7 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

14149019 PMID: 11931850

Structure-activity relationships for inhibition of human 5alpha-reductases by polyphenols.

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Biochemical pharmacology (England) Mar 15 2002, 63 (6) p1165-76, ISSN 0006-2952 Journal Code: 0101032

Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

The enzyme steroid 5 alpha-reductase (EC 1.3.99.5) catalyzes the NADPH-dependent reduction of the double bond of a variety of 3-oxo-Delta(4) steroids including the conversion of testosterone to 5 alpha-dihydrotestosterone. In humans, 5 alpha-reductase activity is critical for certain aspects of male sexual differentiation, and may be involved in the development of benign prostatic hyperplasia, alopecia, hirsutism, and prostate cancer. Certain natural products contain components that are inhibitors of 5 alpha-reductase, such as the green tea catechin

9/AB/5 (Item 5 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

14742236 PMID: 12695345
Enzymology of methylation of tea catechins and inhibition of catechol-O-methyltransferase by (-)-**epigallocatechin gallate**.
Lu Hong; Meng Xiaofeng; Yang Chung S
Department of Chemical Biology, Ernest Mario School of Pharmacy, Rutgers, the State University of New Jersey, Piscataway, New Jersey 08854, USA.
Drug metabolism and disposition- the biological fate of chemicals (United States) May 2003, 31 (5) p572-9, ISSN 0090-9556 Journal Code: 9421550
Contract/Grant No.: CA 56673; CA; NCI; CA88961; CA; NCI
Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed
(-)-Epigallocatechin gallate (EGCG) and (-)-epigallocatechin (EGC) are the major polyphenolic constituents in green tea. In this study, we characterized the enzymology of cytosolic **catechol** -O-methyltransferase (COMT)-catalyzed methylation of EGCG and EGC in humans, mice, and rats. At 1 microM, EGCG was readily methylated by liver cytosolic COMT to 4"-O-methyl-EGCG and then to 4',4"-di-O-methyl-EGCG; EGC was methylated to 4'-O-methyl-EGC. The K(m) and V(max) values for EGC methylation were higher than EGCG; for example, with human liver cytosol, the K(m) were 4.0 versus 0.16 microM and V(max) were 1.28 versus 0.16 nmol/mg/min. Rat liver cytosol had higher COMT activity than that of humans or mice. The small intestine had lower specific activity than the liver in the methylation of EGCG and EGC. Glucuronidation on the B-ring or the D-ring of EGCG greatly inhibited the methylation on the same ring, but glucuronidation on the A-ring of EGCG or EGC did not affect their methylation. Using EGC and 3,4-dihydroxy-L-phenylalanine as substrates, EGCG, 4"-O-methyl-EGCG, and 4',4"-di-O-methyl-EGCG were all potent inhibitors (IC(50) approximately 0.2 microM) of COMT. The COMT-inhibiting activity of (-)-EGCG-3'-O-glucuronide was similar to EGCG, but (-)-EGCG-4"-O-glucuronide was less potent. The present work provides basic information on the methylation of EGCG and suggests that EGCG may inhibit COMT-catalyzed methylation of endogenous and exogenous compounds.

9/AB/6 (Item 6 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

14709393 PMID: 12653203
Synthesis, structure-activity relationship and in vitro evaluation of coelenterazine and coelenteramine derivatives as inhibitors of lipid peroxidation.
Burton Maggi; De Tollenaere Catherine; Cavalier Jean-Francois; Marchand Cecile; Dussart Frederique; Marchand-Brynaert Jacqueline; Rees Jean-Francois
Laboratory of Cell Biology, Institut des Sciences de la Vie, Universite Catholique de Louvain, Place Croix du Sud, 5, B-1348 Louvain-la-Neuve, Belgium.
Free radical research (England) Feb 2003, 37 (2) p145-58, ISSN 1071-5762 Journal Code: 9423872
Publishing Model Print

or 3.12-12.5 mg/L EGCg to amphotericin B 0.125 or 0.25 mg/L (below MIC) at pH 7.0 resulted in enhancement, respectively, of the antifungal effect of amphotericin B against amphotericin B-susceptible or -resistant C. albicans. Combined treatment with 3.12-12.5 mg/L EGCg plus amphotericin B 0.5 mg/L (below MIC) markedly decreased the growth of amphotericin B-resistant C. albicans. When fluconazole-susceptible C. albicans was treated with 25-50 mg/L EGCg and fluconazole 0.125-0.25 mg/L (below MIC), its growth was inhibited by 93.0%-99.4% compared with its growth in the presence of fluconazole alone. The combined use of 12.5 mg/L EGCg and fluconazole 10-50 mg/L (below MIC) inhibited the growth of fluconazole-resistant C. albicans by 98.5%-99.7%. CONCLUSIONS: These results indicate that EGCg enhances the antifungal effect of amphotericin B or fluconazole against antimycotic-susceptible and -resistant C. albicans. Combined treatment with catechin allows the use of lower doses of antimycotics and induces multiple antifungal effects. It is hoped that this may help to avoid the side effects of antimycotics.

9/AB/4 (Item 4 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

15094052 PMID: 14600287

Epigallocatechin gallate modulates CYP450 isoforms in the female Swiss-Webster mouse.

Goodin Mette G; Rosengren Rhonda J

Department of Pharmacology and Toxicology, University of Otago, Dunedin, New Zealand.

Toxicological sciences - an official journal of the Society of Toxicology (United States) Dec 2003, 76 (2) p262-70, ISSN 1096-6080
Journal Code: 9805461
Publishing Model Print-Electronic
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed

This study was designed to determine the effect of the in vivo administration of epigallocatechin gallate (EGCG) and epicatechin gallate (ECG) on enzymes involved in the synthesis and metabolism of estradiol. EGCG (12.5, 25, or 50 mg/kg/day, i.p.) or ECG (12.5 or 25 mg/kg/day, i.p.) was administered to female Swiss-Webster mice for 7 days. The chemicals were well tolerated by the mice with the exception of EGCG given at 50 mg/kg, which resulted in severe hepatic necrosis and a 67% mortality rate. Following the administration of nontoxic doses of EGCG and ECG, aromatase (CYP19), CYP3A, CYP1A, and **catechol** O-methyltransferase (COMT) were measured. Additionally, the activity of CYP2E1 was determined, since this CYP450 isoform is important in the bioactivation of numerous carcinogens. The results demonstrated that ovarian aromatase activity was inhibited 56% by EGCG (25 and 12.5 mg/kg), but not ECG, while hepatic CYP3A catalytic activity and polypeptide levels were increased 31 +/- 4 and 47 +/- 2%, respectively, by 25 mg/kg of EGCG. However, ECG (but not EGCG) inhibited CYP1A catalytic activity and polypeptide levels (31 +/- 5 and 47 +/- 5%, respectively). Hepatic and renal COMT, as well as renal CYP3A remained unchanged following catechin dosing. Hepatic CYP2E1 catalytic activity and polypeptide levels were significantly increased (37 +/- 3 and 22 +/- 3%) following administration of EGCG (25 mg/kg). These results indicate that EGCG modulates enzymes responsible for both the synthesis and metabolism of estradiol, which may provide a potential mechanism for the reported action of EGCG, reported action as an inhibitor of breast tumor growth.

16087621 PMID: 15285844
Inhibition of P-glycoprotein function by tea catechins in KB-C2 cells.
Kitagawa Shuji; Nabekura Tomohiro; Kamiyama Shizu
Niigata University of Pharmacy and Applied Life Sciences, Kamishin'ei-cho 5-13-2, 950-2081, Japan. kitagawa@niigata-pharm.ac.jp
Journal of pharmacy and pharmacology (England) Aug 2004, 56 (8) p1001-5, ISSN 0022-3573 Journal Code: 0376363
Publishing Model Print
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed
We studied the effects of tea catechins, (-)-epicatechin (EC), (-)-epigallocatechin (EGC), (-)-epicatechin gallate (ECG), and (-)-epigallocatechin gallate (EGCG) on the P-glycoprotein (P-gp) function in multidrug-resistant P-gp over-expressing KB-C2 cells. EC did not have any effects on cellular accumulation of P-gp substrates, rhodamine-123 and daunorubicin, but the other catechins increased the accumulation in the order of EGC < ECG < EGCG. The effects of EGCG were larger than those of verapamil and quercetin. Since these catechins inhibited the efflux of P-gp substrates, the elevation of substrate accumulation seemed to be induced by the inhibition of the efflux transporter. The results showed that the inhibitory effects of the catechins did not depend on their total hydrophobicity, but significantly depended on their chemical structure. The presence of the galloyl moiety on the C-ring markedly increased the n-octanol/PBS partition coefficients of the catechins and their activity on P-gp. On the other hand, the presence of the trihydric pyrogallol group as the B-ring decreased the partition coefficients but increased the activity on P-gp, compared with the action of the corresponding catechins with a dihydric **catechol** B-ring.

9/AB/3 (Item 3 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

15179662 PMID: 14688042
Multiple effects of green tea catechin on the antifungal activity of antimycotics against Candida albicans.
Hirasawa Masatomo; Takada Kazuko
Department of Microbiology, Nihon University School of Dentistry at Matsudo, 2-870-1 Sakaecho-nishi, Matsudo City, Chiba 271-8587, Japan. masahira@mascat.nihon-u.ac.jp
Journal of antimicrobial chemotherapy (England) Feb 2004, 53 (2) p225-9, ISSN 0305-7453 Journal Code: 7513617
Publishing Model Print-Electronic
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: MEDLINE; Completed
OBJECTIVES: The susceptibility of Candida albicans to catechin under varying pH conditions and the synergism of the combination of catechin and antimycotics were evaluated.Method: Antifungal activity was determined by broth dilution and calculation of cfu. RESULTS: The antifungal activity of catechin was pH dependent. The concentration of epigallocatechin gallate (EGCg) causing 90% growth inhibition of tested strains of C. albicans was 2000 mg/L at pH 6.0, 500-1000 mg/L at pH 6.5 and 15.6-250 mg/L at pH 7.0. Among catechins, pyrogallol catechin showed stronger antifungal activity against C. albicans than **catechol** catechin. The addition of 6.25-25

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>>>'-' not allowed after set or accession number
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Set     Items   Description
S6       8485   EPIGALLOCATECHIN?
S7       5857   S6(W)GALL?
S8        115   S7(S)CATECHOL?
S9         33   RD (unique items)
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?
? T S9/3 AB/1-33

 9/AB/1     (Item 1 from file: 155)
DIALOG(R)File 155:MEDLINE(R)
(c) format only 2005 Dialog. All rts. reserv.

17878731   PMID: 15808422
  Structure-activity relationship of the tocopherol-regeneration reaction
by catechins.
  Mukai Kazuo; Mitani Shuji; Ohara Keishi; Nagaoka Shin-Ichi
  Department of Chemistry, Faculty of Science, Ehime University, Matsuyama
790-8577, Japan. mukai@chem.sci.ehime-u.ac.jp
  Free radical biology & medicine (United States) May 1 2005, 38 (9)
 p1243-56, ISSN 0891-5849   Journal Code: 8709159
  Publishing Model Print
  Document type: Journal Article
  Languages: ENGLISH
  Main Citation Owner: NLM
  Record type: In Process
  The reaction rates (k(r)) of 5,7-diisopropyl-tocopheroxyl radical (Toc)
with catechins (epicatechin (EC), epicatechin gallate (ECG),
epigallocatechin (EGC), epigallocatechin gallate (EGCG)) and related
compounds (methyl gallate (MG), 4-methylcatechol (MC), and
5-methoxyresorcinol (MR)) have been measured by stopped-flow
spectrophotometer. The k(r) values increased in the order of MR < < MG < EC
< MC approximately ECG < EGC < EGCG in ethanol and 2-propanol/H(2)O (5/1,
v/v) solutions, indicating that the reactivity of the OH groups in
catechins increased in the order of resorcinol A-ring < < gallate G-ring <
catechol B-ring < pyrogallol B-ring. The catechins which have lower
oxidation potentials show higher reactivities. The rate constants for
catechins in micellar solution showed notable pH dependence with one or two
peaks around pH 9-11, because of the dissociation of various phenolic
hydroxyl protons in catechins. The structure-activity relationship in the
free-radical-scavenging reaction by catechins has been clarified by the
detailed analyses of the pH dependence of k(r) values. The reaction rates
increased remarkably with increasing the anionic character of catechins,
that is, the electron-donating capacity of catechins. The mono anion form
at catechol B-and resorcinol A-rings and dianion form at pyrogallol
B-and gallate G-rings show the highest activity for
free-radical-scavenging. It was found that catechins (EC, ECG, EGC, and
EGCG) have activity similar to or higher than that of vitamin C in vitamin
E regeneration at pH 7-12 in micellar solution.


 9/AB/2     (Item 2 from file: 155)
DIALOG(R)File 155:MEDLINE(R)
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File 155:MEDLINE(R) 1951-2005/Aug W2
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Set     Items   Description
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S7       5857   S6(W)GALL?
S8        115   S7(S)CATECHOL?
S9         33   RD (unique items)
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 1/AB/1     (Item 1 from file: 73)
DIALOG(R)File  73:EMBASE
(c) 2005 Elsevier Science B.V. All rts. reserv.

12426814     EMBASE No: 2004023814
  Enzymatic synthesis of tea theaflavin derivatives and their
anti-inflammatory and cytotoxic activities
  Sang S.; Lambert J.D.; Tian S.; Hong J.; Hou Z.; Ryu J.-H.; Stark R.E.;
Rosen R.T.; Huang M.-T.; Yang C.S.; Ho C.-T.
  S. Sang, Department of Chemical Biology, Ernest Mario School of Pharmacy,
  Rutgers University, 164 Frelinghuysen Road, Piscataway, NJ 08854-8020
  United States
  AUTHOR EMAIL: ssang@rci.rutgers.edu
  Bioorganic and Medicinal Chemistry ( BIOORG. MED. CHEM. ) (United Kingdom
  )   15 JAN 2004, 12/2 (459-467)
  CODEN: BMECE   ISSN: 0968-0896
  DOCUMENT TYPE: Journal ; Article
  LANGUAGE: ENGLISH   SUMMARY LANGUAGE: ENGLISH
  NUMBER OF REFERENCES: 43

  Derivatives based on a benzotropolone skeleton (9-26) have been prepared
by the enzymatic coupling (horseradish peroxidase/HSUB2OSUB2) of selected
pairs of compounds (1-8), one with a vic-trihydroxyphenyl moiety, and the
other with an ortho-dihydroxyphenyl structure. Some of these compounds have
been found to inhibit TPA-induced mice ear edema, nitric oxide (NO)
synthesis, and arachidonic acid release by LPS-stimulated RAW 264.7 cells.
Their cytotoxic activites against KYSE 150 and 510 human esophageal
squamous cell carcinoma and HT 29 human colon cancer cells were also
evaluated. (c) 2003 Elsevier Ltd. All rights reserved.
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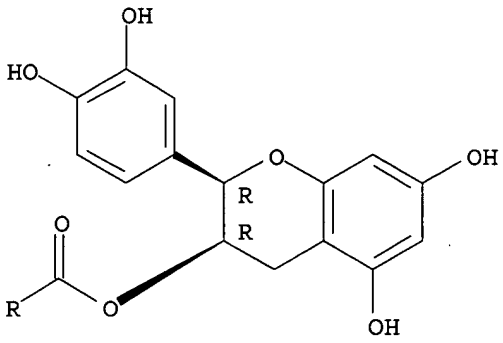
PAGE 2-A



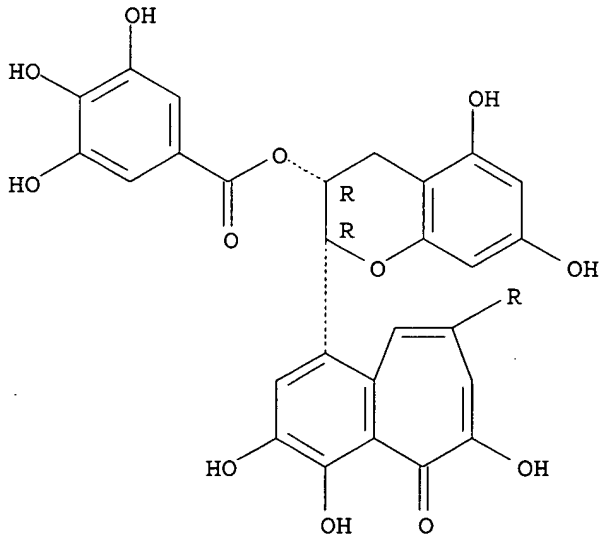
pigments
AUTHOR(S): Bailey, R. G.; Nursten, H. E.; McDowell, I.
CORPORATE SOURCE: Dep. Food Sci. Technol., Univ. Reading, Reading, RG6 2AP, UK
SOURCE: Journal of the Science of Food and Agriculture (1993), 63(4), 455-64
CODEN: JSFAAE; ISSN: 0022-5142
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The chemical oxidation of polyphenols has been used to produce black tea pigments. (+)-Catechin, (-)-epicatechin, (-)-epicatechin gallate and (-)-epigallocatechin gallate were isolated from convenient sources, their identity being confirmed by mass spectrometry and HPLC. The oxidation of a mixture of (-)-epicatechin gallate and gallic acid gave an oxidation product of (-)-epicatechin gallate in addition to epitheaflavic acid 3-gallate. The catechins were oxidized chemical and the products analyzed by HPLC, the chromatograms being compared with a black tea chromatogram. The reactions gave both resolved and unresolved pigments, and many of the resolved pigments had HPLC retention times close to black tea pigments. Each catechin behaved differently, the chromatograms of the oxidation products from each starting material being clearly distinguishable. Resolved pigments were obtained by the chemical oxidation of other phenolic compds. This work provides a convenient method for studying the formation of resolved and unresolved black tea pigments.

IT **152542-70-6**
RL: BIOL (Biological study)
(catechin oxidation product)
RN 152542-70-6 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



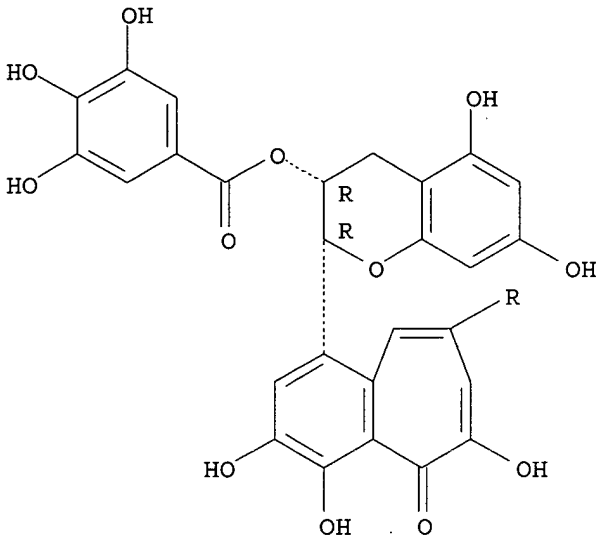
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(new type of tea pigment, theaflavate A, from the chemical oxidation of epicatechin gallate and isolated from tea)

RN 152542-70-6 HCAPLUS

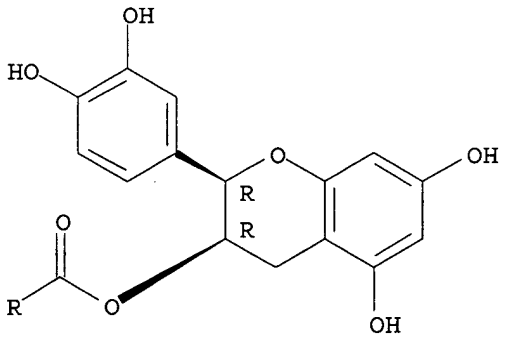
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



L27 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN

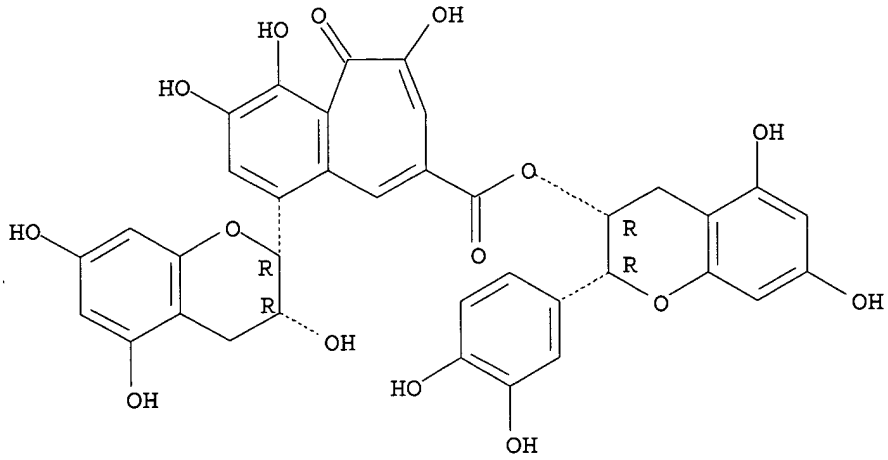
ACCESSION NUMBER: 1994:75969 HCAPLUS

DOCUMENT NUMBER: 120:75969

TITLE: The chemical oxidation of catechins and other phenolics: a study of the formation of black tea

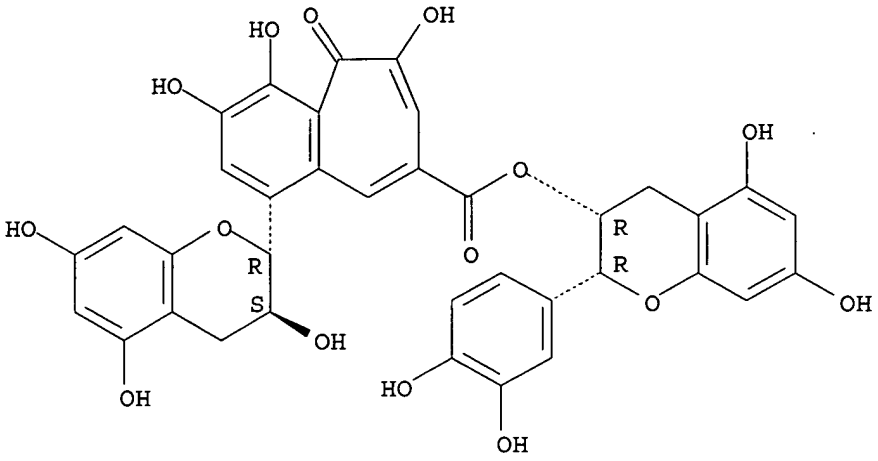
RN 220473-65-4 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:462161 HCAPLUS
DOCUMENT NUMBER: 127:160922
TITLE: A new type of tea pigment - from the chemical oxidation of epicatechin gallate and isolated from tea
AUTHOR(S): Wan, Xiaochun; Nursten, Harry E.; Cai, Ya; Davis, Adrienne L.; Wilkins, John P. G.; Davies, Alan P.
CORPORATE SOURCE: Dep. Food Sci. Technol., Univ. Reading, Reading, RG6 6AP, UK
SOURCE: Journal of the Science of Food and Agriculture (1997), 74(3), 401-408
CODEN: JSFAAE; ISSN: 0022-5142
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB (-)-Epicatechin-3-O-gallate (ECG), one of the major green tea polyphenols, was oxidized chemical using potassium ferricyanide. The major oxidation product, termed theaflavate A, which gave a sharp peak on HPLC anal., was separated and purified by a combination of chromatog. on Sephadex LH-10 and a semi-preparative HPLC method. This compound was characterized by NMR spectroscopy (1H, 13C, HMQC, HMMBC, and ROESY) and mass spectrometry (electrospray method) and was found to have a novel benzotropolone skeleton formed between the B-ring of one ECG mol. and the galloyl ester group of another. Compds. containing this type of benzotropolone link were also found to be present in black tea. This benzotropolone link is of great interest, since it shows that the galloyl ester groups of flavan-3-ols participate in oxidative condensation reactions. This illustrates the complexity of theaflavin-type compds. in black tea and provides an addnl. reaction pathway for the formation of thearubigins which has not been previously considered.
IT **152542-70-6P**, Theaflavate A



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

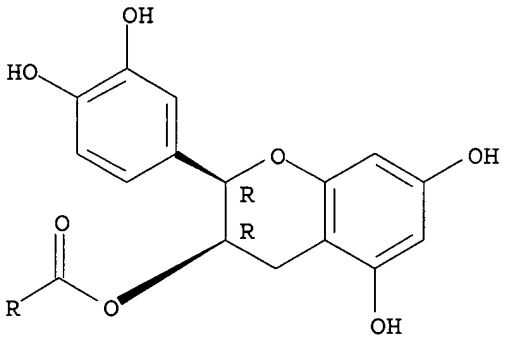
L27 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:37783 HCAPLUS
DOCUMENT NUMBER: 130:168128
TITLE: Theaflavate B, isotheaflavin-3'-O-gallate and neotheaflavin-3-O-gallate: three polyphenolic pigments from black tea
AUTHOR(S): Lewis, John R.; Davis, Adrienne L.; Cai, Ya; Davies, Alan P.; Wilkins, John P. G.; Pennington, Michael
CORPORATE SOURCE: Unilever Research, Colworth Laboratory, Bedford, MK44 1LQ, UK
SOURCE: Phytochemistry (1998), 49(8), 2511-2519
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Three new polyphenolic compds., theaflavate B (I), isotheaflavin-3'-O-gallate (II) and neotheaflavin-3-O-gallate (III), have been characterized in exts. from black tea (the fermented leaves of Camellia sinensis). The structures of these compds. were determined using 1D and 2D NMR spectroscopy, mass spectrometry and chemical oxidation of catechin precursors. Theaflavate B contains a benzotropolone moiety produced from oxidation of the galloyl ester group of a flavan-3-O-gallate and as such represents a new class of polyphenol pigments obtained from black tea.

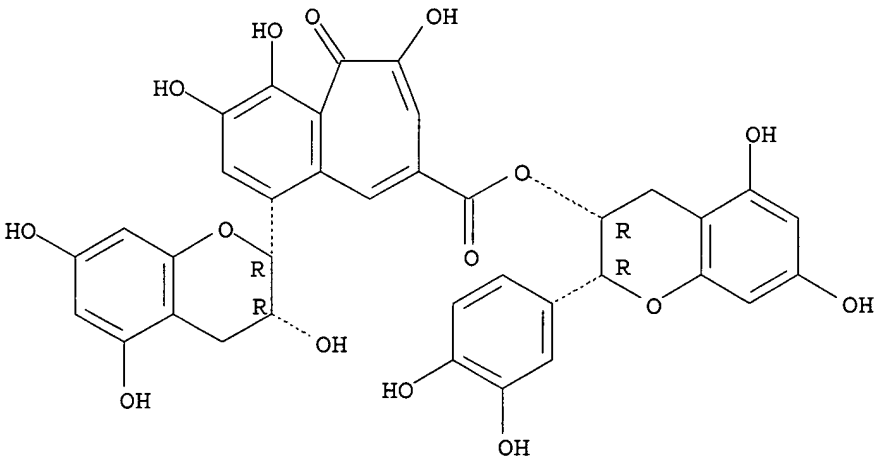
IT **220473-65-4P**, Theaflavate B
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation, structure and synthesis of theaflavate B, isotheaflavin-3'-O-gallate and neotheaflavin-3-O-gallate, polyphenolic pigments from black tea)

PAGE 2-A



RN 220473-65-4 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 691399-24-3 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Derivs. based on a benzotropolone skeleton (9-26) have been prepared by the enzymic coupling (horseradish peroxidase/H2O2) of selected pairs of compds. (1-8), one with a vic-trihydroxyphenyl moiety, and the other with an ortho-dihydroxyphenyl structure. Some of these compds. have been found to inhibit TPA-induced mice ear edema, nitric oxide (NO) synthesis, and arachidonic acid release by LPS-stimulated RAW 264.7 cells. Their cytotoxic activities against KYSE 150 and 510 human esophageal squamous cell carcinoma and HT 29 human colon cancer cells were also evaluated.

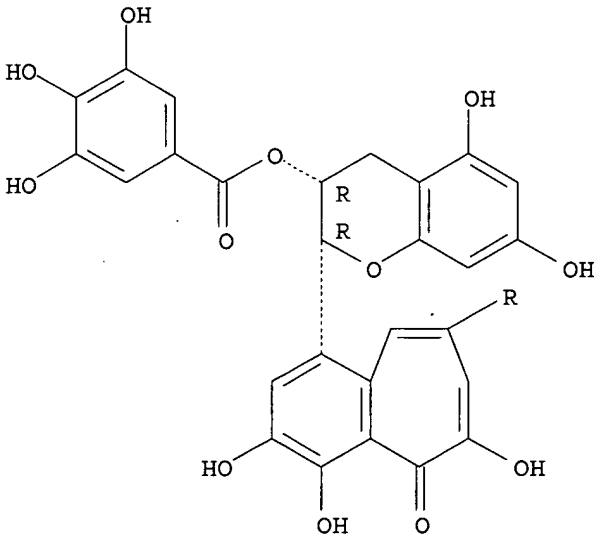
IT **152542-70-6P**, Theaflavate A **220473-65-4P**, Theaflavate B **691399-24-3P**, Neotheaflavate B
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzymic synthesis of tea theaflavin derivs. and their anti-inflammatory and cytotoxic activities)

RN 152542-70-6 HCAPLUS

CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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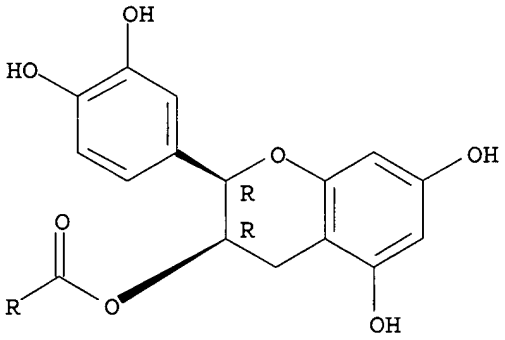
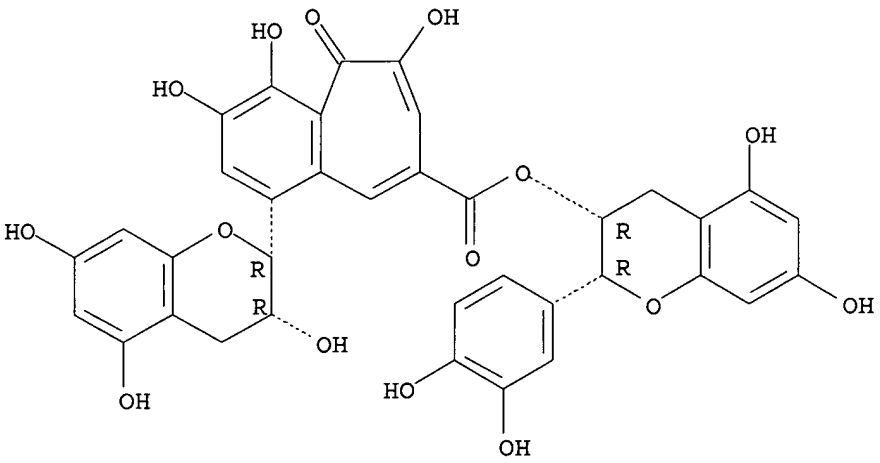


RN 220473-65-4 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:34784 HCAPLUS
DOCUMENT NUMBER: 140:417534
TITLE: Enzymatic synthesis of tea theaflavin derivatives and their anti-inflammatory and cytotoxic activities
AUTHOR(S): Sang, Shengmin; Lambert, Joshua D.; Tian, Shiying; Hong, Jungil; Hou, Zhe; Ryu, Jae-He; Stark, Ruth E.; Rosen, Robert T.; Huang, Mou-Tuan; Yang, Chung S.; Ho, Chi-Tang
CORPORATE SOURCE: Ernest Mario School of Pharmacy, Department of Chemical Biology, Rutgers University, Piscataway, NJ, 08854-8020, USA
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(2), 459-467
CODEN: BMECEP; ISSN: 0968-0896

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Black tea contains 2 major groups of pigments, theaflavins (TFs) and thearubigins (TRs). TFs contain a bis-flavan substituted 1,2-dihydroxy-3,4-benzotropolone moiety. Unlike the TFs, TRs have not yet been characterized. The chemical structure of the TRs remains a mystery. The present paper reports the effort to study the structure of TFs and TRs using delayed pulsed ion extraction of ions generated via the matrix-assisted laser desorption ionization (MALDI) technique, on line with a Linear time-of-flight (TOF) mass spectrometer. Spectra of standard TFs show not only pseudomol. ions but also ions resulting from fragmentation. The anal. of MALDI-TOF spectra of black tea fractions shows the structure of some TRs, which are similar to those of TFs because the same loss of mass is observed

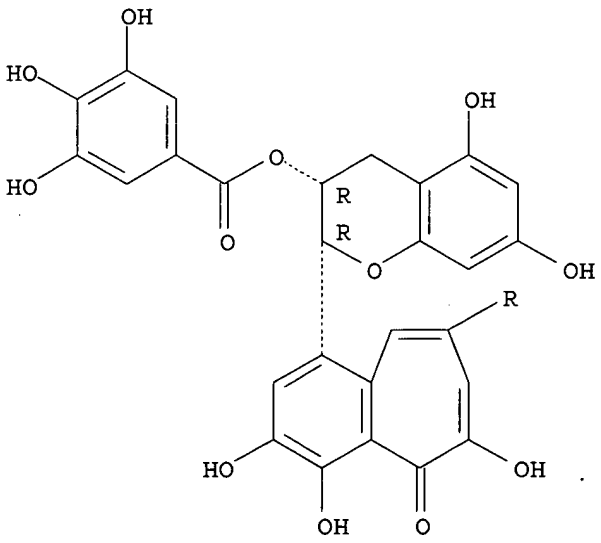
IT **152542-70-6**, Theaflavate A **220473-65-4**, Theaflavate B
RL: ANT (Analyte); ANST (Analytical study)
(anal. of theaflavins and thearubigins from black tea extract by MALDI-TOF MS)

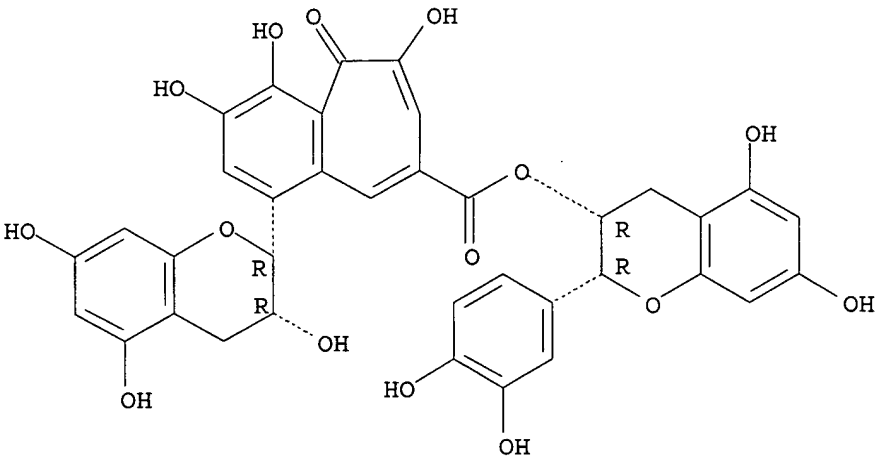
RN 152542-70-6 HCAPLUS

CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

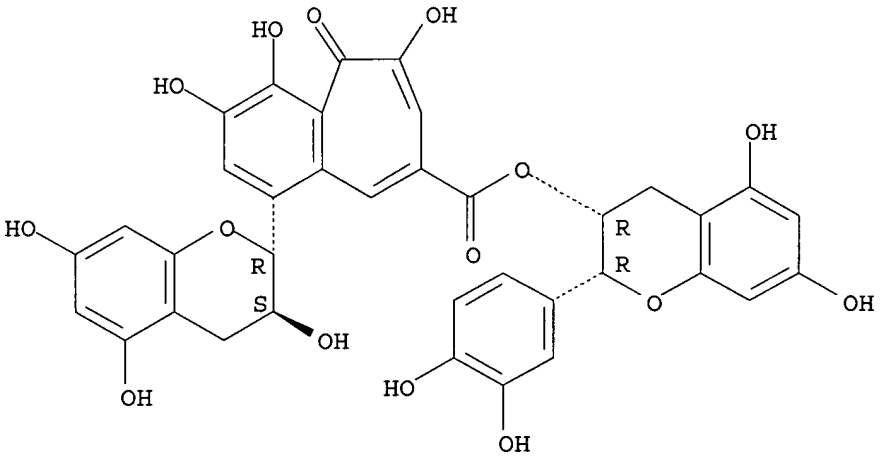
PAGE 1-A





RN 691399-24-3 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

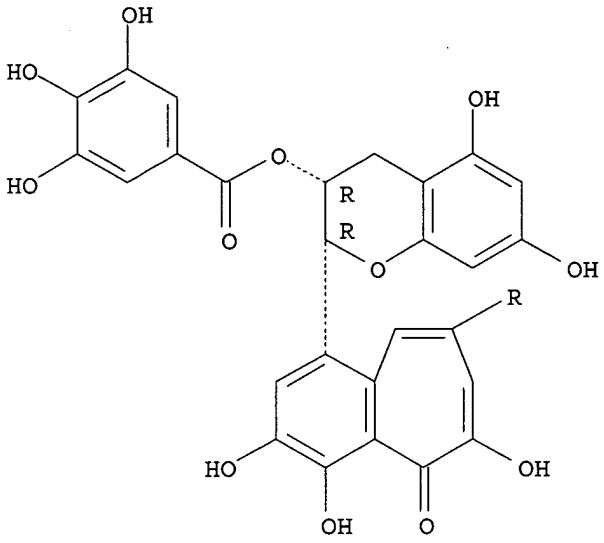


L27 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:264111 HCAPLUS
DOCUMENT NUMBER: 140:420055
TITLE: Analysis of Theaflavins and Thearubigins from Black Tea Extract by MALDI-TOF Mass Spectrometry
AUTHOR(S): Menet, Marie-Claude; Sang, Shengmin; Yang, Chung S.; Ho, Chi-Tang; Rosen, Robert T.
CORPORATE SOURCE: Department of Food Science and Center for Advanced Food Technology, Rutgers University, New Brunswick, NJ, 08901-8520, USA
SOURCE: Journal of Agricultural and Food Chemistry (2004), 52(9), 2455-2461
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society

trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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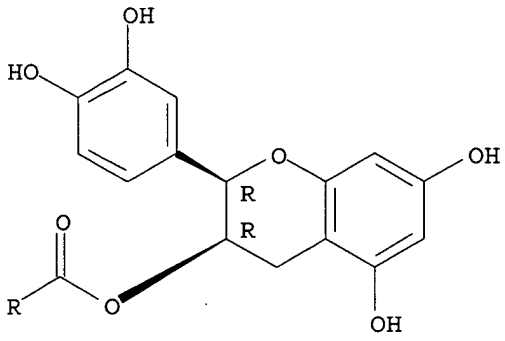


RN 220473-65-4 HCAPLUS

CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

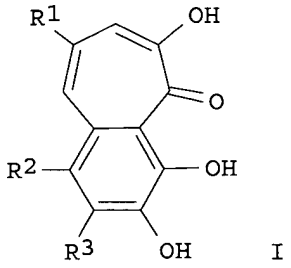
Absolute stereochemistry.

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005049284	A1	20050303	US 2003-652813	20030829
WO 2005021479	A1	20050310	WO 2004-US28164	20040830

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-652813 A 20030829
OTHER SOURCE(S): MARPAT 142:261331
GI



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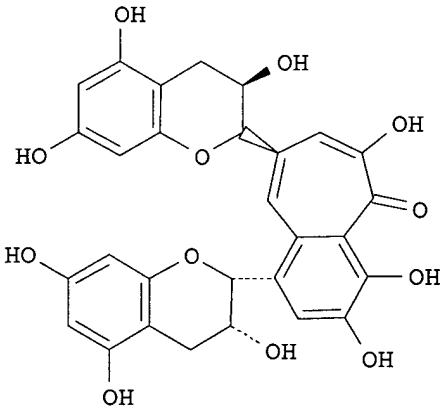
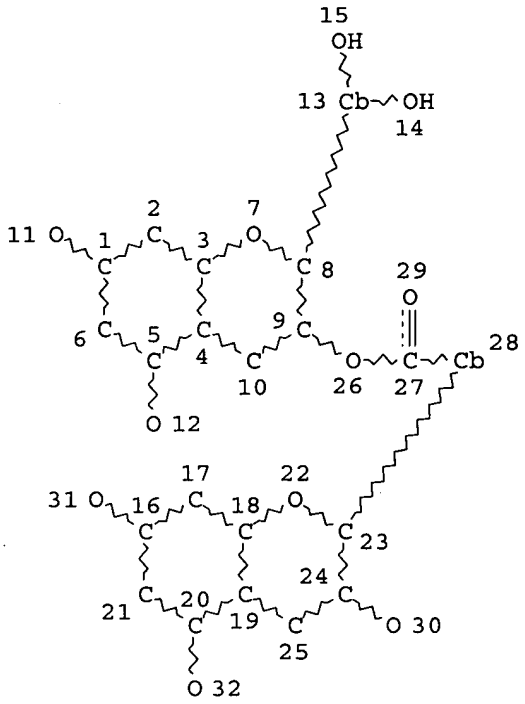


II

AB The present invention discloses novel method of synthesizing benzotropolone compds., such as I [R1, R2, R3 = H, OH, alkoxy, alkyl, aryl, indolyl, Ph, benzyl, pyridinyl, pyrrolyl, thiophenyl], a salt or an ester of thereof, for their use as antioxidant and antiinflammatory agents. Thus, (-)-epicatechin and (-)-epigallocatechin were dissolved in a mixture of acetone-pH 5.0 phosphate citrate buffer containing horseradish peroxidase, and treated with H2O2 to afford theaflavin (II). II exhibit relative oxygen-radical absorbance capacity (ORAC) value 11.60 ± 0.30.

IT **152542-70-6P**, Theaflavate A **220473-65-4P**, Theaflavate B **691399-24-3P**, Neotheaflavate B
RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(enzymic synthesis of benzotropolone derivs. as antioxidants and antiinflammatory agents)

RN 152542-70-6 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-3,4,6-



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 32

STEREO ATTRIBUTES: NONE
L26 3 SEA FILE=REGISTRY SUB=L24 SSS FUL L25
L27 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L26

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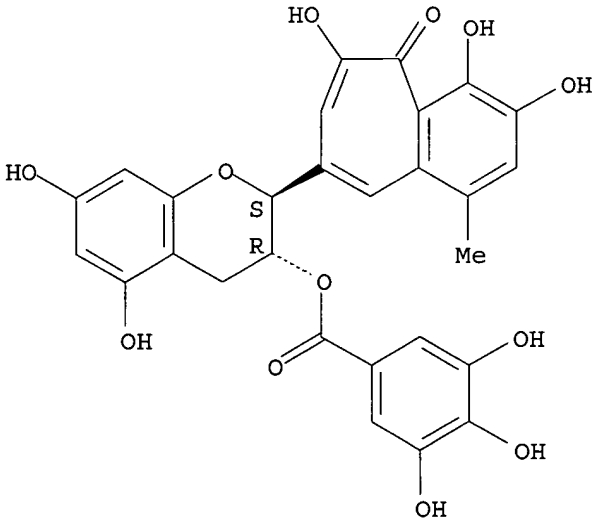
L27 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:185391 HCAPLUS
DOCUMENT NUMBER: 142:261331
TITLE: Preparation of benzotropolone derivatives as antioxidants and anti-inflammatory agents
INVENTOR(S): Ho, Chi-Tang; Ghai, Geetha; Sang, Shengmin; Jhoo, Jin-Woo; Huang, Mou-Tuan; Rosen, Robert T.; Dushenkov, Slavik
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent



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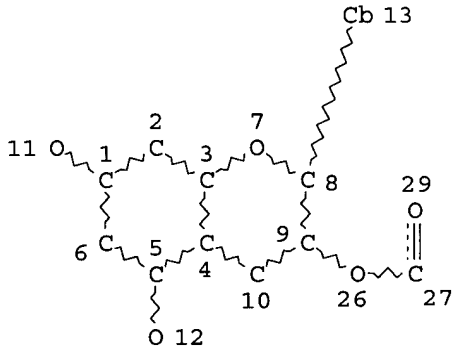

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NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
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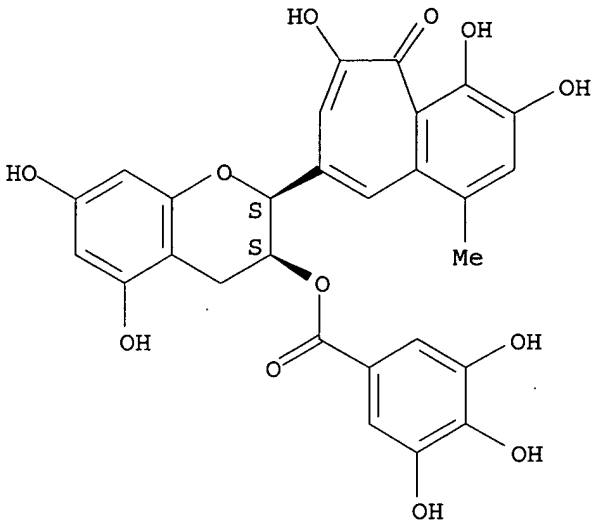
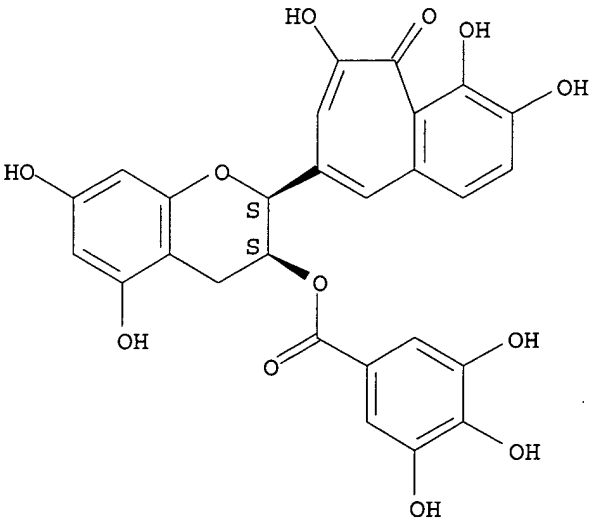


RN 41002-00-0 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,6-trihydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

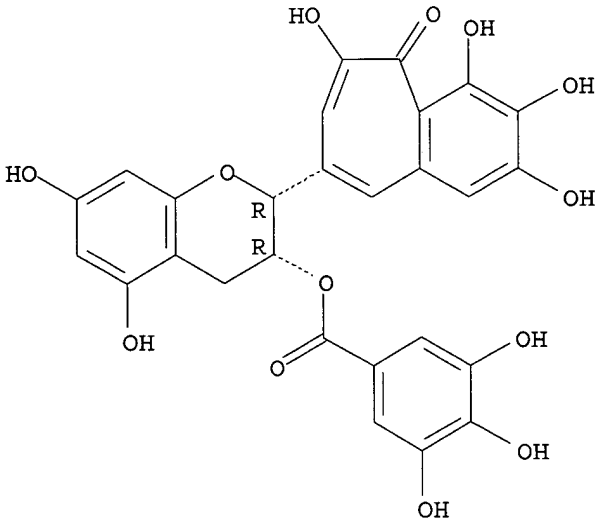


RN 41002-01-1 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,6-trihydroxy-1-methyl-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

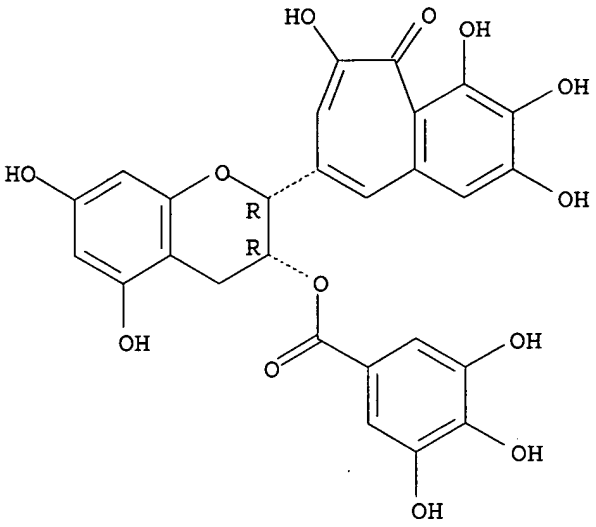
(of black tea)
RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

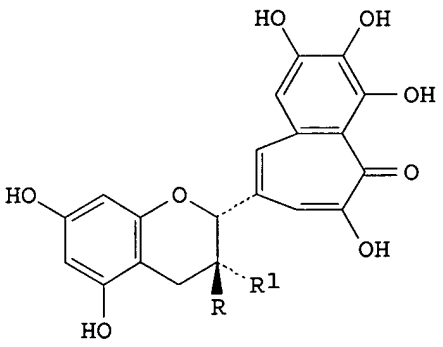


L17 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:124409 HCAPLUS
DOCUMENT NUMBER: 78:124409
TITLE: Theaflavins of black tea
AUTHOR(S): Collier, P. D.; Bryce, T.; Mallows, R.; Thomas, P. E.; Frost, D. J.; Korver, O.; Wilkins, C. K.
CORPORATE SOURCE: Unilever Res. Lab., Sharnbrook, UK
SOURCE: Tetrahedron (1973), 29(1), 125-42
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Eight pigments were isolated from the theaflavin fraction of black tea and their structures, relative configurations, and precursors determined The principal pigments were theaflavin (I), its 3- and 3'monogallates, and the 3,3'-digallate. The steric hindrance to rotation of the flavan groups in these and monoflavan-substituted model compds. were correlated with NMR data. The 3-gallate and 3,3'-digallate existed in rotameric forms, which were observed in the temperature-dependent CD spectra .
IT **41001-98-3 41002-00-0 41002-01-1**
RL: PRP (Properties)
(spectrum of)
RN 41001-98-3 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, 3,4-dihydro-5,7-dihydroxy-2-(3,4,6-trihydroxy-1-methyl-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L17 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:203856 HCAPLUS
DOCUMENT NUMBER: 104:203856
TITLE: Tannins and related compounds. XXXVI. Isolation and structures of theaflagallins, new red pigments from black tea
AUTHOR(S): Nonaka, Genichiro; Hashimoto, Fumio; Nishioka, Itsuo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ. 62, Fukuoka, 812, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1986), 34(1), 61-5
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I, R=H, R^1=O-B-D-gluco
II, R=H, R^1=OH
III, R=OH, R^1=H

AB Black tea (Camellia sinensis assamica) polyphenols contained 3 new red pigments, epitheaflagallin 3-O-gallate (I), epitheaflagallin (II), and theaflagallin (III), together with known theaflavins. The structures of the theaflagallins (I, III, III) were determined by spectroscopic and chemical data as unusual benzotropolones formed by oxidative condensation of gallic acid and so-called gallocatechins.
IT **102067-92-5**
RL: BIOL (Biological study)

(-)-epigallocatechin 3-O-gallate and novel dimeric flavan-3-ols, oolonghomobisflavans A and B, from oolong tea. (3)

AUTHOR(S): Hashimoto, Fumio; Nonaka, Genichiro; Nishioka, Itsuo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1989), 37(12), 3255-63
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:196860
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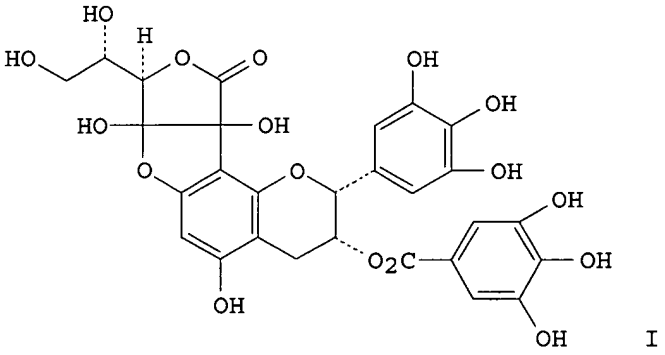


I

AB A chemical examination of the polyphenolic constituents in com. oolong tea led to the isolation of 32 compds., including a new flavan-3-ol, 2 novel dimeric flavan-3-ols named oolonghomobisflavans A and B, and 8 new proanthocyanidins, together with 21 known polyphenols, including proanthocyanidins, hydrolyzable tannins, and red pigments. On the basis of chemical and spectroscopic evidence, the flavan-3-ol was characterized as 8-C-ascorbyl (-)-epigallocatechin 3-O-gallate (I), and oolonghomobisflavans A and B were determined to be dimeric flavan-3-ols in which 2 units were linked through a methylene bridge at the 8,8'- and 8,6'-positions, resp. The structures of the new proanthocyanidins were elucidated, mainly by tannase hydrolysis and thiolytic degradation, to be epicatechin-(4β→8)-epigallocatechin 3-O-gallate, epicatechin 3-O-gallate-(4β→8)-epigallocatechin 3-O-gallate, catechin-(4α→8)-epigallocatechin 3-O-gallate, prodelphinidin B-4 3'-O-gallate, epicatechin 3-O-gallate-(4β→6)-epigallocatechin 3-O-gallate, epigallocatechin 3-O-gallate-(4β→6)-epicatechin 3-O-gallate, epi-afzelechin 3-O-gallate-(4β→6)-epigallocatechin 3-O-gallate, and prodelphinidin B-2 3'-O-gallate.

IT **102067-92-5**
RL: BIOL (Biological study)
(of oolong tea)

RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

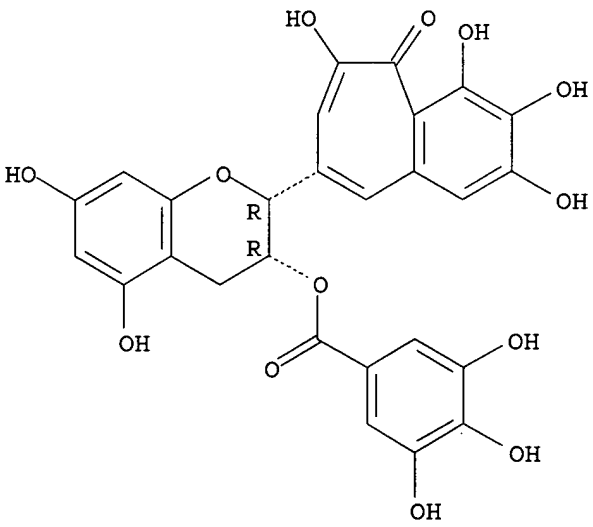
TITLE: Tannins and related compounds. CXIV. Structures of novel fermentation products, theogallinin, theaflavonin and desgalloyl theaflavonin from black tea, and changes of tea leaf polyphenols during fermentation
AUTHOR(S): Hashimoto, Fumio; Nonaka, Genichiro; Nishioka, Itsuo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1992), 40(6), 1383-9
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three novel fermentation products, theogallinin (I), theaflavonin (II), and desgalloyl theaflavonin were isolated from black tea. The structure of I was established on the basis of physicochem. evidence to be a condensation product linked through pyrogallol-pyrogallol rings in theogallin and (-)-epigallocatechin 3-O-gallate (III), while II and desgalloyl II were characterized as B,B'-linked bisflavonoids formed by an oxidative coupling of isomyricitrin and tea catechins [III and (-)-epigallocatechin]. Furthermore, HPLC analyses of the changes of tea polyphenols during fermentation have revealed that original tea catechins are more rapidly transformed by endogenous phenol oxidase to theasinensins (e.g. theasinensins A and C) and oolongtheanin than the known black tea pigments, theaflavins.

IT **102067-92-5**, Epitheaflagallin 3-O-gallate
RL: BIOL (Biological study)
(of tea leaf, during fermentation)

RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



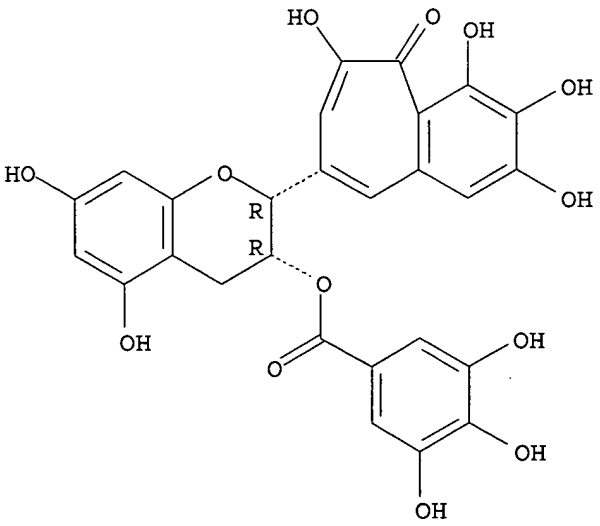
L17 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:196860 HCAPLUS
DOCUMENT NUMBER: 112:196860
TITLE: Tannins and related compounds. XC. 8-C-ascorbyl

L17 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:190224 HCAPLUS
DOCUMENT NUMBER: 124:331679
TITLE: Anti-AIDS agents. 24. Evaluation of tea polyphenols as anti-HIV agents
AUTHOR(S): Hashimoto, Fumio; Kashiwada, Yoshiki; Nonaka, Genichiro; Nishioka, Itsuo; Nohara, Toshihiro; Cosentino, L. Mark; Lee, Kuo-Hsiung
CORPORATE SOURCE: Sch. Pharmacy, Univ. North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(6), 695-700
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Thirty-eight tea polyphenols were evaluated for their inhibitory effect against HIV replication in H9 lymphocyte cells. 8-C-ascorbyl-(-)-epigallocatechin and theasinensin-D demonstrated relatively potent anti-HIV activity with EC50 values of 4 and 8 μg/mL and therapeutic indexes of 9.5 and 5, resp.

IT **102067-92-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(evaluation of tea polyphenols as anti-HIV agents)
RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:37880 HCAPLUS
DOCUMENT NUMBER: 118:37880

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:562816 HCAPLUS
DOCUMENT NUMBER: 133:172213
TITLE: Catechin derivatives as matrix metalloprotease (MMP) inhibitors for treatment of MMP-related diseases
INVENTOR(S): Akizawa, Toshifumi; Yahara, Shoji; Hashimoto, Fumio; Yamada, Masashi; Suma, Sachie; Kono, Tetsuya; Uchida, Katsuyuki; Oshiba, Yukio
PATENT ASSIGNEE(S): Meiji Milk Products, Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

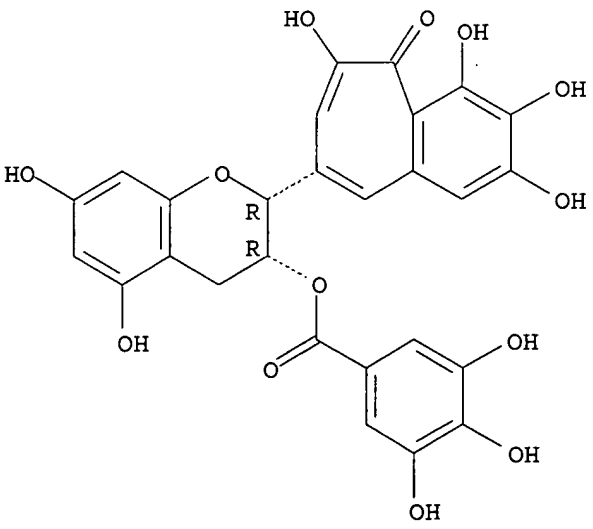
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000226329	A2	20000815	JP 1999-192268	19990706
PRIORITY APPLN. INFO.:			JP 1998-359996 A	19981204

AB Catechin derivs. e.g. theasinensin A, F, D, and G, oolongtheanin 3'-O-gallate, assamicain A, etc. are claimed as matrix metalloprotease (MMP) inhibitors for treatment of MMP-related diseases, including chronic rheumatoid arthritis, periodontal disease, tumor metastasis, vascular diseases, HIV infections , diabetic complications, etc.

IT **102067-92-5**, Epitheaflagallin 3-O-gallate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(catechin derivs. as matrix metalloprotease (MMP) inhibitors for treatment of MMP-related diseases)

RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



TITLE: Evaluation of the anti-oxidative effect (in vitro) of tea polyphenols

AUTHOR(S): Hashimoto, Fumio; Ono, Masateru; Masuoka, Chikako; Ito, Yasuyuki; Sakata, Yusuke; Shimizu, Keiichi; Nonaka, Gen-Ichiro; Nishioka, Itsuo; Nohara, Toshihiro

CORPORATE SOURCE: Faculty of Agriculture, Kagoshima University, Korimoto 1-21-24, Kagoshima, 890-0065, Japan

SOURCE: Bioscience, Biotechnology, and Biochemistry (2003), 67(2), 396-401
CODEN: BBBIEJ; ISSN: 0916-8451

PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

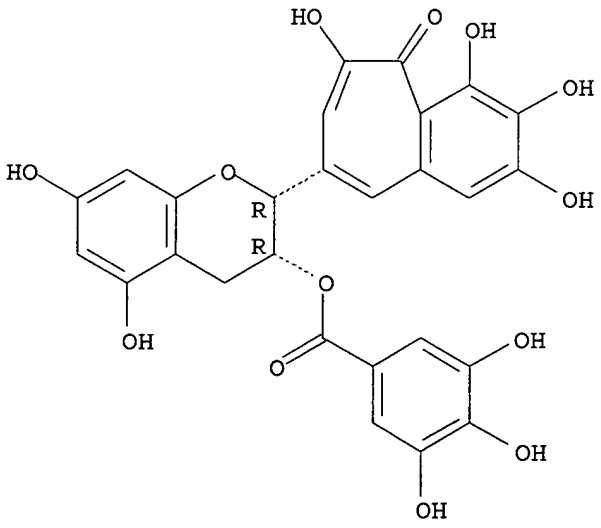
AB Forty-three polyphenols from tea leaves were evaluated for their anti-oxidative effect against lipid peroxidn. by the ferric thiocyanate method in vitro. Among these, 1,4,6-tri-O-galloyl-β-D-glucose (hydrolyzable tannin) showed the highest anti-oxidative activity against lipid peroxidn., even stronger than that of 3-tert.-butyl-4-hydroxyanisole (BHA). The assay demonstrates that tea polyphenols, except for desgalloylated dimeric proanthocyanidins that possess a catechin structure in the upper unit and desgalloylated flavan-3-ols, and excepting theaflavin 3,3'-di-O-gallate, had more anti-oxidative activity than that of α-tocopherol. The chemical structure-activity relationship shows that the anti-oxidative action advanced with the condensation of two mols. of flavan-3-ols as well as with 3-O-acylation in the flavan skeleton such as that by galloyl, (3'-O-methyl)-galloyl, and p-coumaroyl groups.

IT **102067-92-5**, Epitheaflagallin 3-O-gallate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(in vitro antioxidative effects of tea polyphenols against lipid peroxidn.)

RN 102067-92-5 HCAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS

the 21st Century, School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, 422-8526, Japan
SOURCE: Biological & Pharmaceutical Bulletin (2003), 26(9), 1235-1238
CODEN: BPBLEO; ISSN: 0918-6158
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

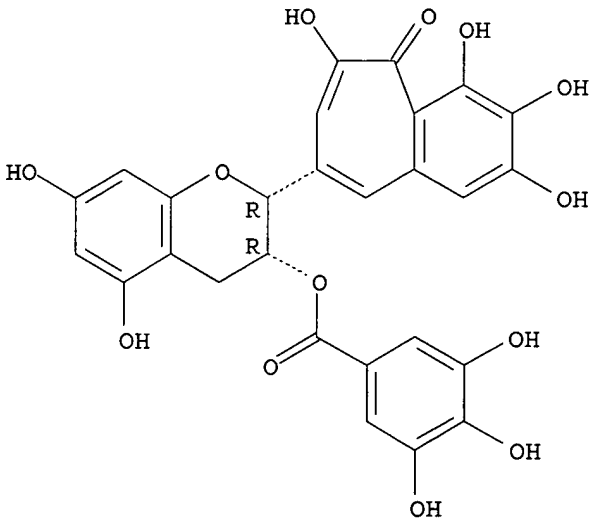
AB Matrix metalloproteinases (MMPs), especially membrane-type 1 matrix metalloproteinase (MT1-MMP), which generates an active form of MMP-2 from proMMP-2, are deeply involved in angiogenesis as well as in tumor cell migration and metastasis. To obtain a specific inhibitor for MT1-MMP, we screened a number of natural and synthetic compds. using recombinant human MMP-2, MMP-7, and soluble MT1-MMP in a fluorogenic peptide cleavage assay. (-)-Epigallocatechin 3-O-gallate (EGCG) followed by (-)-epigallocatechin 3,5-di-O-gallate and epitheaflagallin 3-O-gallate, was found to have potent and distinct inhibitory activity against MT1-MMP. Therefore, we investigated the effect of EGCG on the suppression of MMP-2 activation as determined by gelatin zymog., and observed that the active form of MMP-2 in the conditioned medium of human umbilical vein endothelial cells was decreased in the presence of EGCG. The results suggest the possibility that tea polyphenols suppress tumor growth through the suppression of angiogenesis.

IT **102067-92-5**, Epitheaflagallin 3-O-gallate
RL: PAC (Pharmacological activity); BIOL (Biological study)
(inhibitory effect of green tea polyphenols on membrane-type 1 matrix metalloproteinase)

RN 102067-92-5 HCAPLUS

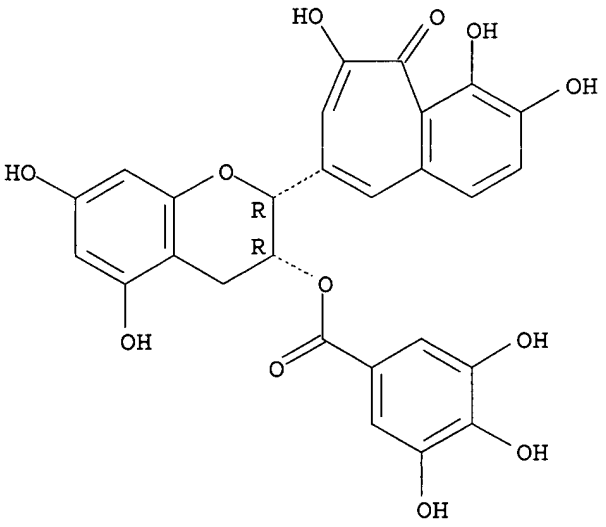
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



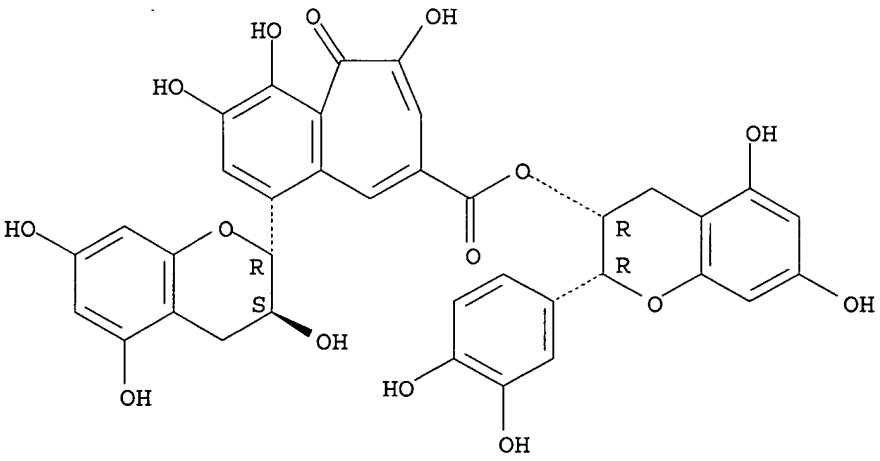
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:193543 HCAPLUS
DOCUMENT NUMBER: 138:367880



RN 691399-24-3 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:745733 HCAPLUS
DOCUMENT NUMBER: 140:210042
TITLE: Inhibitory effect of green tea polyphenols on membrane-type 1 matrix metalloproteinase, MT1-MMP
AUTHOR(S): Oku, Naoto; Matsukawa, Motomi; Yamakawa, Satoru; Asai, Tomohiro; Yahara, Shoji; Hashimoto, Fumio; Akizawa, Toshifumi
CORPORATE SOURCE: Department of Medical Biochemistry and COE Program in

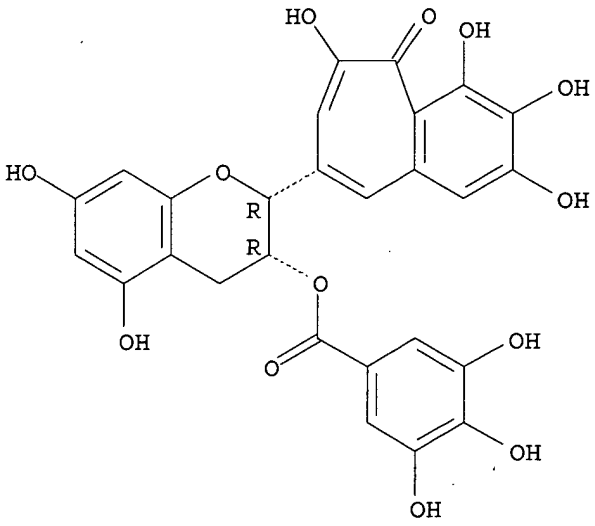
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Derivs. based on a benzotropolone skeleton (9-26) have been prepared by the enzymic coupling (horseradish peroxidase/H2O2) of selected pairs of compds. (1-8), one with a vic-trihydroxyphenyl moiety, and the other with an ortho-dihydroxyphenyl structure. Some of these compds. have been found to inhibit TPA-induced mice ear edema, nitric oxide (NO) synthesis, and arachidonic acid release by LPS-stimulated RAW 264.7 cells. Their cytotoxic activities against KYSE 150 and 510 human esophageal squamous cell carcinoma and HT 29 human colon cancer cells were also evaluated.

IT **102067-92-5P 691378-77-5P 691399-24-3P,**
Neotheaflavate B
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzymic synthesis of tea theaflavin derivs. and their anti-inflammatory and cytotoxic activities)

RN 102067-92-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 691378-77-5 HCAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,6-trihydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004359576	A2	20041224	JP 2003-157862	20030603

PRIORITY APPLN. INFO.: JP 2003-157862 20030603

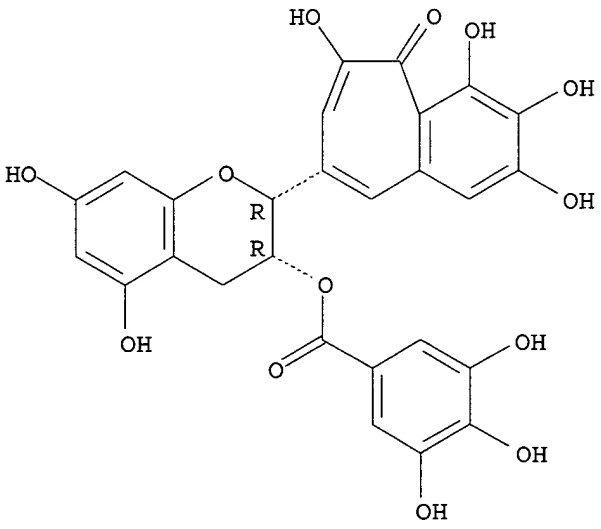
AB Purpurogallin derivs. , including theaflavin derivs., from red tea exts. are claimed as HL-60 tumor cell apoptosis inducers and health foods for treatment of human acute promyelocytic leukemia. The antitumor effects of the purpurogallin derivs. were tested in vitro.

IT **102067-92-5**, Epitheaflagallin 3-O-gallate
RL: DMA (Drug mechanism of action); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(purpurogallin derivs. from red tea exts. as HL-60 tumor cell apoptosis inducers)

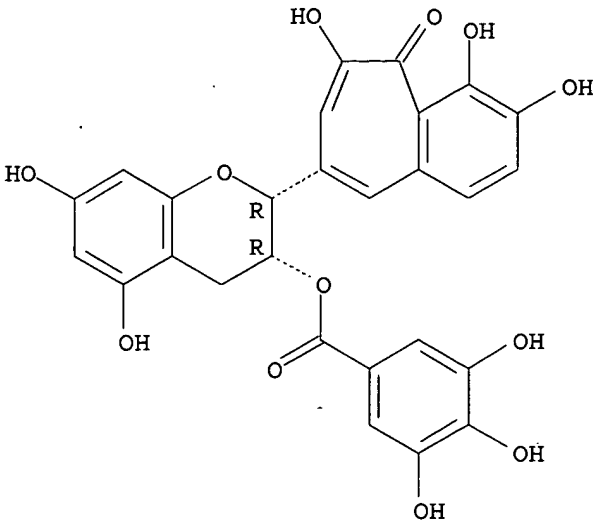
RN 102067-92-5 HCAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(2,3,4,6-tetrahydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

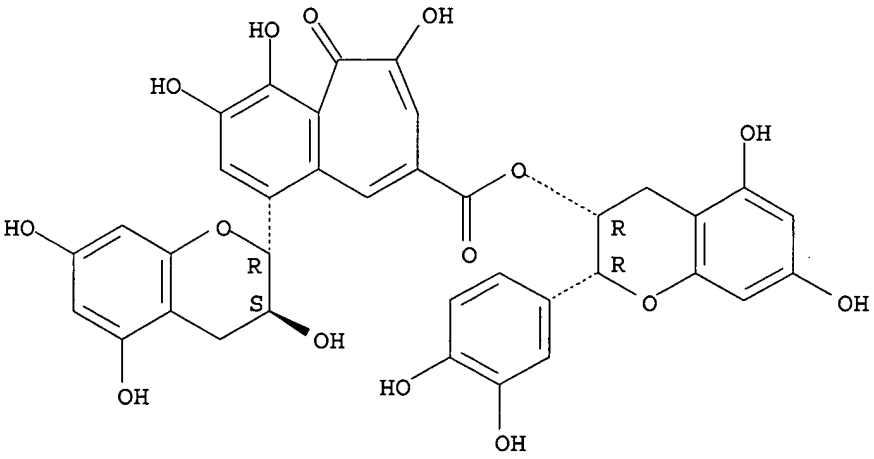


L17 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:34784 HCAPLUS
DOCUMENT NUMBER: 140:417534
TITLE: Enzymatic synthesis of tea theaflavin derivatives and their anti-inflammatory and cytotoxic activities
AUTHOR(S): Sang, Shengmin; Lambert, Joshua D.; Tian, Shiying; Hong, Jungil; Hou, Zhe; Ryu, Jae-He; Stark, Ruth E.; Rosen, Robert T.; Huang, Mou-Tuan; Yang, Chung S.; Ho, Chi-Tang
CORPORATE SOURCE: Ernest Mario School of Pharmacy, Department of Chemical Biology, Rutgers University, Piscataway, NJ, 08854-8020, USA
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(2), 459-467



RN 691399-24-3 HCAPLUS
CN 5H-Benzocycloheptene-8-carboxylic acid, 1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1128645 HCAPLUS
DOCUMENT NUMBER: 142:32948
TITLE: Purpurogallin derivatives from red tea extracts as HL-60 tumor cell apoptosis inducers
INVENTOR(S): Hou, Te-Hsing; Hashimoto, Fumio; Fujii, Makoto; Sakata, Yusuke
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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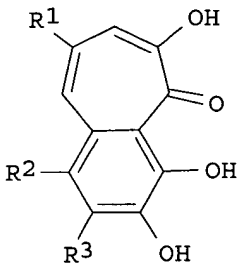
PRIORITY APPLN. INFO.: US 2003-652813 A 20030829
OTHER SOURCE(S): MARPAT 142:261331

GI



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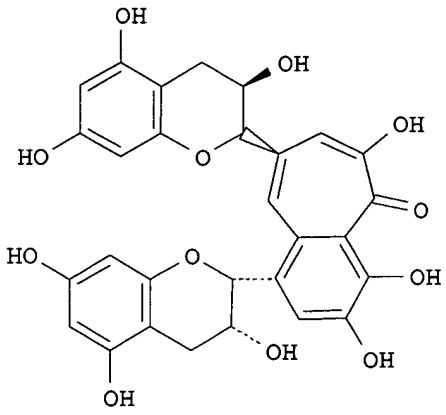


II

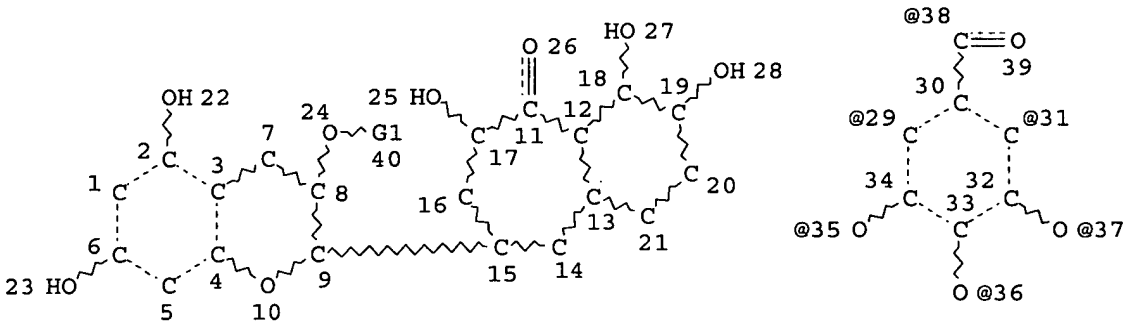
AB The present invention discloses novel method of synthesizing benzotropolone compds., such as I [R1, R2, R3 = H, OH, alkoxy, alkyl, aryl, indolyl, Ph, benzyl, pyridinyl, pyrrolyl, thiophenyl], a salt or an ester of thereof, for their use as antioxidant and antiinflammatory agents. Thus, (-)-epicatechin and (-)-epigallocatechin were dissolved in a mixture of acetone-pH 5.0 phosphate citrate buffer containing horseradish peroxidase, and treated with H2O2 to afford theaflavin (II). II exhibit relative oxygen-radical absorbance capacity (ORAC) value 11.60 ± 0.30.

IT **691378-77-5P 691399-24-3P, Neotheaflavate B**
RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(enzymic synthesis of benzotropolone derivs. as antioxidants and antiinflammatory agents)

RN 691378-77-5 HCAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,6-trihydroxy-5-oxo-5H-benzocyclohepten-8-yl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

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L17 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:185391 HCAPLUS
DOCUMENT NUMBER: 142:261331
TITLE: Preparation of benzotropolone derivatives as antioxidants and anti-inflammatory agents
INVENTOR(S): Ho, Chi-Tang; Ghai, Geetha; Sang, Shengmin; Jhoo, Jin-Woo; Huang, Mou-Tuan; Rosen, Robert T.; Dushenkov, Slavik
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005049284	A1	20050303	US 2003-652813	20030829
WO 2005021479	A1	20050310	WO 2004-US28164	20040830

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

=> FIL HCAPLUS
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FILE COVERS 1907 - 17 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 16 Aug 2005 (20050816/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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substance identification.

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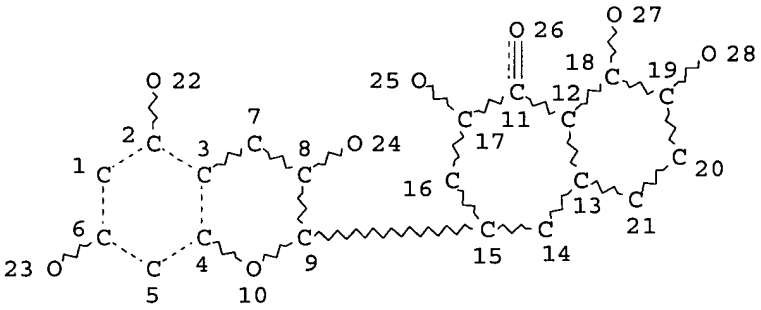
L1 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE
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* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
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Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE HCAPLUS

FILE COVERS 1907 - 17 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 16 Aug 2005 (20050816/ED)

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L25             STR L18
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                D IBIB ABS HITSTR L27 1-6

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     FILE REGISTRY
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     provided by InfoChem.

     STRUCTURE FILE UPDATES:   16 AUG 2005  HIGHEST RN 860495-66-5
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     TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     ************************************************************
     *                                                          *
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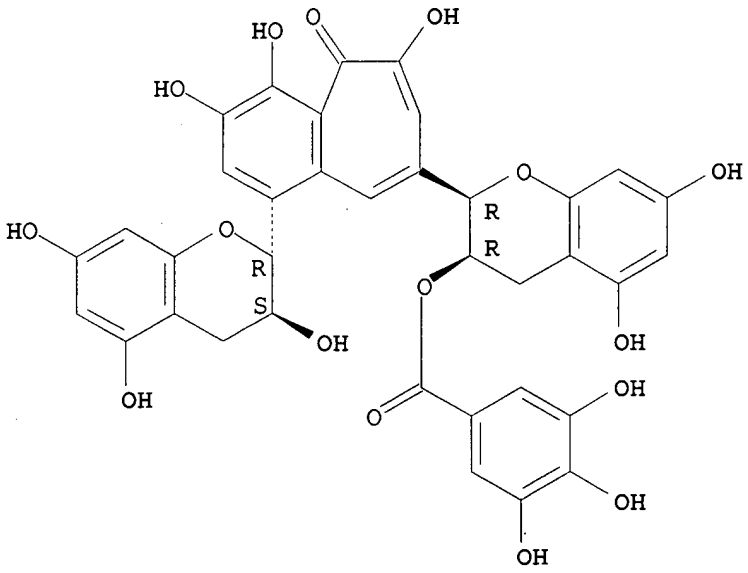
L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:37783 CAPLUS
DOCUMENT NUMBER: 130:168128
TITLE: Theaflavate B, isotheaflavin-3'-O-**gallate** and neotheaflavin-3-O-**gallate**: three polyphenolic pigments from black **tea**
AUTHOR(S): Lewis, John R.; Davis, Adrienne L.; Cai, Ya; Davies, Alan P.; Wilkins, John P. G.; Pennington, Michael
CORPORATE SOURCE: Unilever Research, Colworth Laboratory, Bedford, MK44 1LQ, UK
SOURCE: Phytochemistry (1998), 49(8), 2511-2519
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **220473-68-7P**, Neotheaflavin 3-O-**gallate**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)
(isolation, structure and synthesis of theaflavate B, isotheaflavin-3'-O-**gallate** and neotheaflavin-3-O-**gallate**, polyphenolic pigments from black **tea**)
RN 220473-68-7 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-2-[1-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy-5-oxo-5H-benzocyclohepten-8-yl]-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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Uploading C:\Program Files\Stnexp\Queries\813.str

L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR
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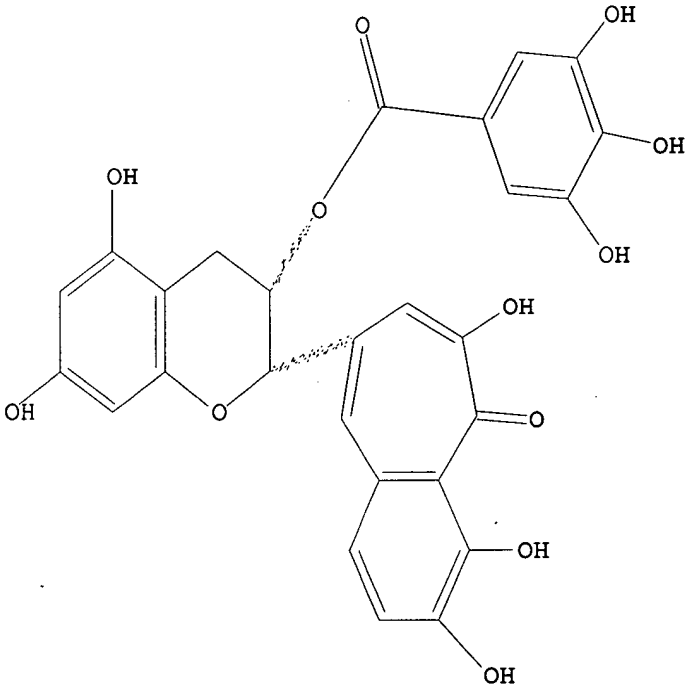


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Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 15:16:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED         1 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:16:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     46 TO ITERATE

100.0% PROCESSED        46 ITERATIONS                               15 ANSWERS
SEARCH TIME: 00.00.01

L3            15 SEA SSS FUL L1

=> d scan
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=> d his

     (FILE 'HOME' ENTERED AT 14:05:15 ON 17 AUG 2005)

     FILE 'HCAPLUS, CAOLD' ENTERED AT 14:05:29 ON 17 AUG 2005
L1         10724 S BENZOTROPOLONE? OR ?CATECHIN
L2           949 S L1 AND (?PEROXIDASE OR ENZYME OR ENZYMATIC)
L3            61 S L2 AND HYDROGEN PEROXIDE
L4            32 S L3 AND (?FLAVIN OR EPIGALLOCATECHIN)
L5             2 S NEOTHEAFLAVATE?
```

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=> d his

     (FILE 'HOME' ENTERED AT 15:15:22 ON 17 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 15:15:31 ON 17 AUG 2005
L1             STRUCTURE UPLOADED
L2               0 S L1
L3              15 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:17:12 ON 17 AUG 2005
L4             208 S L3
L5               0 S L4 AND (EPIGALLOCATECHINOCATECHOL GALLATE OR EGCGC?)
L6             189 S L4 AND (GALLATE OR GALLIC ACID)
L7             110 S L6 AND CATECHIN?
L8              97 S L7 AND TEA
L9               2 S L8 AND BENZOTROPOLONE?
L10              2 S L8 AND INFLAMMAT?
L11             97 S L8 AND GALLATE
L12              2 S L11 AND HYDROGEN PEROXIDE
L13             14 S L11 AND ANTIOXIDANT
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=> d his

     (FILE 'HOME' ENTERED AT 12:05:45 ON 26 AUG 2005)

     FILE 'HCAPLUS, CAOLD' ENTERED AT 12:05:56 ON 26 AUG 2005
L1           144 S BENZOTROPOLONE?
L2         26216 S ?CATECHIN? OR GALLIC ACID OR GALLATE
L3            27 S L1 AND L2
L4         10592 S PYROGALLOL
L5          1773 S L4 AND CATECHOL
L6             3 S L3 AND L5
L7             5 S L3 AND (PEROXIDASE OR POLYPHENOL OXIDASE)
L8             2 S L7 AND HYDROGEN PEROXIDE

     FILE 'BIOSIS, MEDLINE' ENTERED AT 12:12:49 ON 26 AUG 2005
L9            25 S BENZOTROPOLONE?
L10           10 S L9 AND (?CATECHIN? OR GALLATE OR GALLIC ACID)
L11            3 S L10 AND (PEROXIDASE OR POLYPHENOL OXIDASE)
L12            1 S L11 AND HYDROGEN PEROXIDE
```

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